Ruđer Bošković Institute

Annual Report 2012

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Ruđer Bošković Institute

Annual Report 2012

Zagreb, 2013.

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TECHNICAL SUPPORT

Design

Centre of Informatics and Computing

Technical Processing

Franjo Matković

Printing

PRINTERA GRUPA d.o.o.

Print run of 500 copies

Web edition

http://www.irb.hr/eng/About-the-RBI/Annual-Reports

ISSN 1334-854X

Contents

Dear reader,

Welcome to the 2012 Annual Report of the Ruđer Bošković Institute. The aim of this report is to provide a succinct overview of the most important activities and top achievements made at the Ruđer Bošković Institute during 2012. As such, the report covers exemplary performance in high-quality fundamental research, published in top journals or scientific books, and shows the strong involvement of scientists of the Ruđer Bošković Institute in higher education. The report also highlights selected awards, recognitions, patents, domestic and international projects and collaborations, important invited lectures, and international conferences organized by the Institute during the year.

On behalf of the Editorial Board, I would like to take this opportunity to sincerely thank the RBI staff for their cooperation during the preparation of this report. We would also like to thank you, the reader, for your interest and take pleasure in inviting you to share with us your comments and suggestions regarding future editions of this report.

Editor
Nela Pivac

Introduction

OVERVIEW

The primary task of the RBI is to conduct excellent basic research, which is a prerequisite for the fulfilment of the other tasks that the RBI assumes in the development of the Republic of Croatia. These include the development of innovative research, participation in higher education, the transfer of knowledge to industry with the goal of developing new high-tech products and increasing public awareness of the importance and necessity of knowledge and science in modern society. The RBI carries out these tasks in collaboration with universities, scientific institutions and other related institutions in Croatia and other countries. The Institute is also strongly engaged in the promotion of the popularization of science through numerous activities such as various series of popular science lectures for the general public, which are traditionally held at the Institute. In 2012, the Institute became active on several social networks, including Facebook, Twitter and Vimeo.

The RBI is most certainly Croatia's most successful institution in securing FP projects. By the end of 2012, the RBI had contracted 24 FP7 projects valued at slightly less than 5 million EUR. There has been a strong emphasis on planning the renewal of the infrastructure of the Institute through the current infrastructure project at the RBI, Open Scientific Infrastructure Platforms for Innovative Applications in the Economy and Society (O-ZIP). The project is valued at approximately € 50 million and its orientation are applications and achieving wider socio-cultural benefits, meaning that all the infrastructure and know-how will be open and available to the wider Croatian scientific, research and technology communities. Apart from O-ZIP, the RBI has partnered with other institutions on three more structural projects, which have found their place on the indicative lists of the relevant ministries, such as the Croatian Centre for Advanced Materials and Nano Technology (in partnership with the University of Zagreb and the Institute of Physics), ZOO (Croatian Scientific and Educational Cloud) in cooperation with Uniersity of Zagreb's Computing Centre (SRCE), as well as the Science Educational Entertainment Centre (SEEC).

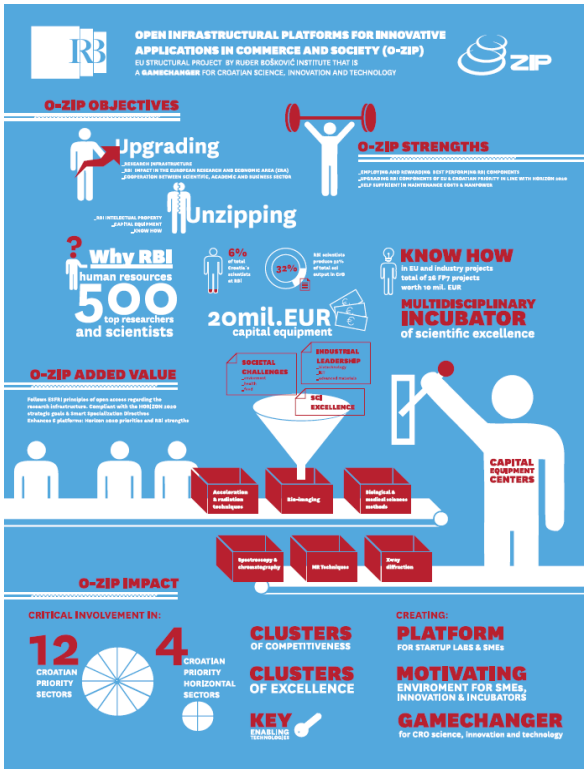


Figure 1. An overview of the RBI's primary structural project – O-ZIP.

The RBI is regarded as Croatia's leading scientific institute in the natural and biomedical sciences as well as marine and environmental research, owing to its size, scientific productivity, international reputation

in research, and the quality of its scientific personnel and research facilities. The Institute is the leading and most internationally competitive Croatian institute by virtue of its participation in international research projects, such as the IPA, IAEA and FP7 program

organic chemistry and biochemistry, molecular biology and medicine, marine science and the environment, information and computer sciences, laser and nuclear research and development. The internal distribution of RBI employees can be seen in table 1.

	RESEARCH STAFF					TECHNICIANS AND STAFF SCIENTISTS	ADMINISTRATIVE STAFF	MAINTAINANCE AND SECURITY	LIBRARY AND IT STAFF	TOTAL
	PERMANENT SCIENTISTS			POST-DOCTORAL FELLOWS	GRADUATE STUDENTS					
	Senior Scientists	Senior Research Associates	Research Associates							
Theoretical Physics Division	6	4	7	2	5	0	1	0	0	25
Division of Experimental Physics	11	11	9	10	15	9	3	1	0	69
Division of Materials Physics	5	6	5	1	7	2	1	0	0	27
Division of Laser and Atomic Research and Development	1	1	2	1	3	13	1	1	0	23
Division of Electronics	5	1	0	2	4	1	0	0	0	13
Division of Physical Chemistry	10	7	9	7	7	10	1	1	0	52
Division of Organic Chemistry and Biochemistry	8	11	15	12	17	10	1	3	0	77
Division of Materials Chemistry	6	6	16	7	5	11	1	2	0	54
Division of Molecular Biology	7	9	14	12	17	8	1	2	0	70
Division of Molecular Medicine	13	6	15	17	16	17	2	2	0	88
Division of Marine and Environmental Research	15	11	22	10	23	17	2	2	0	102
Centre for Marine Research	5	10	9	3	10	9	1	6	0	53
Centre for Informatics and Computing	1	0	2	0	3	0	0	0	6	12
Centre for Nuclear Magnetic Resonance	3	4	2	0	3	4	0	0	0	16
Library	0	0	0	0	0	0	0	0	10	10
Administration	0	1	0	0	1	7	47	26	0	82
Technical services	0	0	0	0	0	0	2	61	0	63
TOTAL	96	88	127	84	136	118	64	107	16	836

Table 1. Internal disitribution of RBI employees

funded by the European Commission, NATO, Cogito, COST, UNESCO and other international scientific foundations. While the RBI constitutes only about 6% of the total scientific community in Croatia, about 30% of the scientific papers and total scientific activities originate from its employees.

There are nearly 900 persons employed at the Institute today. Over 550 of them are scientists and researchers that pursue research in more than 80 laboratories in theoretical and experimental physics, material physics and chemistry, electronics, physical chemistry,

ORGANIZATION OF THE INSTITUTE

Organizationally, the RBI consists of twelve divisions, two centres, a library, the office of the Director General, as well as sections for maintenance and technical services and administration (Figure 2).

The administrative structure of the Institute sees central roles of the Board of Governors, the Director General and the Scientific Council. An important input is derived from the Heads of the Divisions and Centres (via their

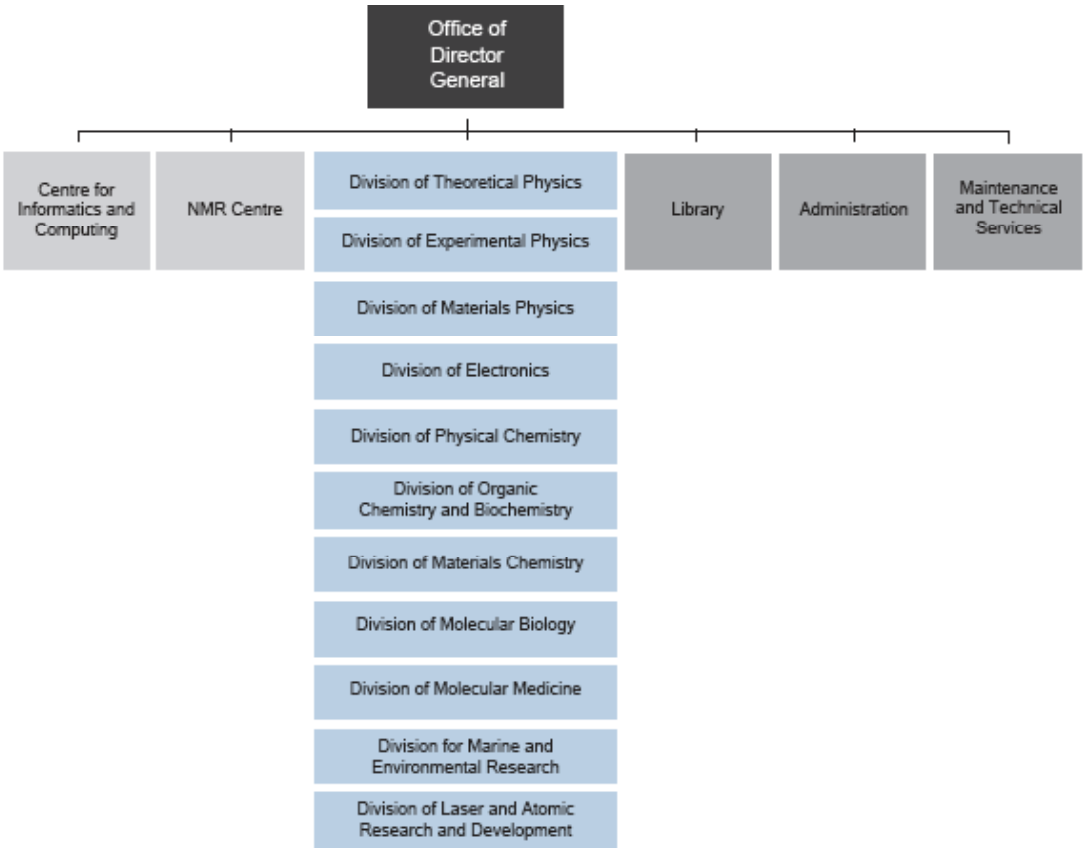


Figure 2. The organizational structure of the RBI.

Divisional Councils), the Assistant Directors, as well as the Heads of the Administration, the Maintenance and Technical Services and the Library (Figure 3). The International advisory board provides vital external advice and guidance.

Director General: Danica Ramljak / Tome Antičić
Head of the Scientific Council: Neven Bilić / Miroslav Plohl
Chairman of the Board of Governors: Slavko Krajcar / Đuro Miljanić

International Scientific Board

Farooq Azam, University of California, USA
Fernando Azorin, Institute of Molecular Biology of Barcelona, Spain
Jonathan R. Ellis, CERN, Switzerland
Joshua Jortner, Tel Aviv University, Israel
Bernd Kaina, Institut für Toxikologie, Germany
Harold Kroto, University of Sussex, UK
Jean-Marie Lehn, Institut de Science et d'Ingénierie Supramoléculaires, France
Thomas C. Malone, University of Maryland Center for Environmental Science, USA
Egon Matijević, Clarkson University, USA
Jutta Ludwig Müller, Institute of Botany, Technische Universität Dresden, Germany
Werner E.G. Müller, Johannes Gutenberg Universität, Germany
A.R. Peaker, University of Manchester, UK
Roberto D. Peccei, University of California Los Angeles, USA
Olivia Pereira-Smith, UT Health Science Center, USA
Nadia Pinardi, University of Bologna, Italy

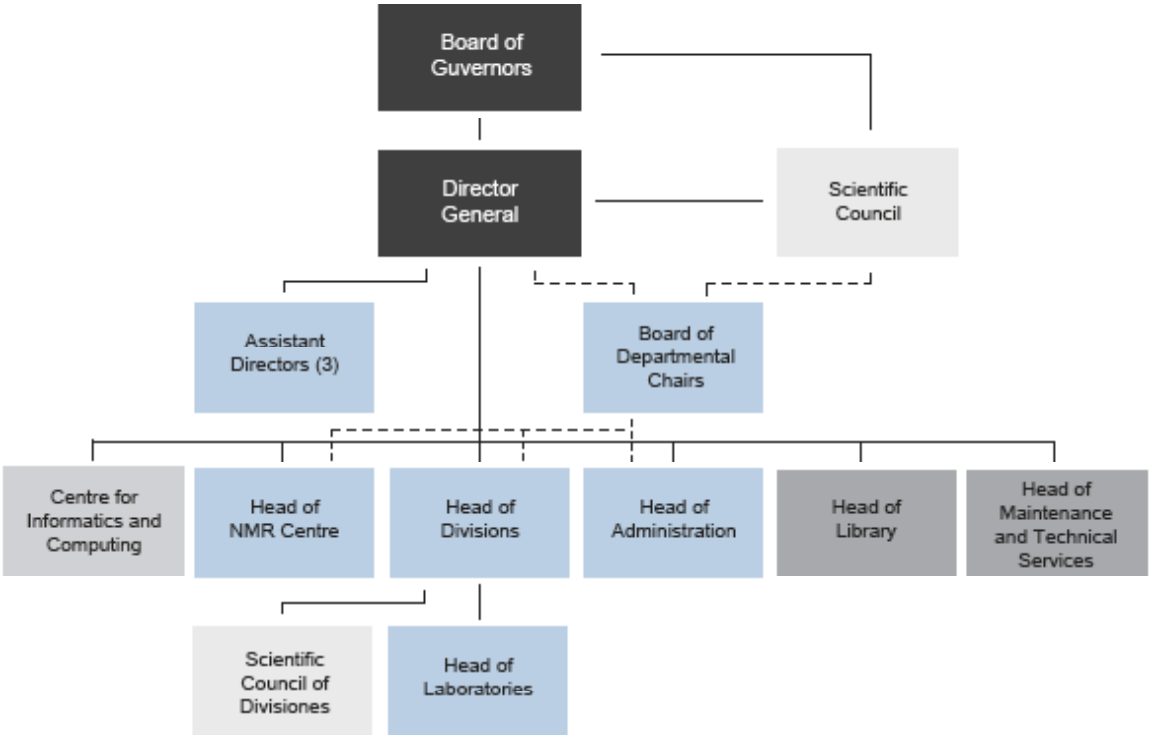


Figure 3. The administrative structure of the RBI

Bogdan Povh, University of Heidelberg, Max-Planck-Institut für Kernphysik, Germany
Miroslav Radman, Université René Descartes-Paris V, France
Joseph Schlessinger, Yale University, USA
Hans Joachim Seitz, Universität Hamburg, Germany
Peter J. Stambrook, University of Cincinnati Medical Center, USA
Rudolf Zechner, Institute for Molecular Biosciences, Austria
Walter Giger, Swiss Federal Institute for Aquatic Sciences and Technology, Switzerland

ACTIVITIES

Fundamental research

The total number of research articles published by RBI scientists in 2012 was 770. Among these, 631 articles were published in journals indexed in WoS, the majority of which were published in high ranking international Journals.

The details of the many important discoveries made by RBI scientists in 2012 are to be found in the subsequent sections of this report. Nevertheless, we present here a small section of highlights in order to convey a general impression of the kind research carried out at the Institute.

RBI scientists Borislav Kovačević and Robert Vianello, together with the late Zvonimir Maksić, from the Group for Quantum Organic Chemistry, published a review article entitled "Advances in Determining the Absolute Proton Affinities of Neutral Organic Molecules in the Gas Phase and Their Interpretation: A Theoretical Account" in Chemical Reviews, which is the journal with the highest impact factor in chemistry (IF = 40 197), holding fifth position on the list of all top-ranked journals according to that criteria.

	STAFF	ARTICLES*						THESES			
									Theses (mentored by RBI staff)		
DEPARTMENT	Research staff**	Articles in journals indexed in WoS	Articles in other journals and chapters in books	Articles in conference proceedings	Total articles	Books	Patents	Ph.D. Theses (written by RBI staff)	Ph.D.	M.Sc.	Total mentored theses
Theoretical Physics Division	23	35	3	4	42						
Division of Experimental Physics	50	197	2	6	205			2	3		3
Division of Materials Physics	24	44	2	3	49			1	1		1
Division of Laser and Atomic Research and Development	8	8		1	9		2				
Division of Electronics	10	3		3	6	1					
Division of Physical Chemistry	40	63	5	6	74			1	2	3	5
Division of Organic Chemistry and Biochemistry	62	87	5	1	93		1	1	3	7	10
Division of Materials Chemistry	40	35	5	3	43			3	3		3
Division of Molecular Biology	59	46	5	1	52	2	1	4	4	11	15
Division of Molecular Medicine	66	76	15	1	92			3	8	10	18
Division for Marine and Environmental Research	79	78	9	11	98			2	2	3	5
Center for Marine Research	37	24	4	2	30			1	1		1
Centre for Informatics and Computing	6	7	4	4	15					2	2
NMR Centre	11	22	3		25						
Library	0	1		3	4						
TOTAL	515	631	97	42	770	3	3	18	27	36	63

* Original scientific papers and review papers in journals/conference proceedings and chapters in books

** Permanent scientists, post-doctoral fellows and graduate students

Table 2. Review of publications for the year 2012

The Group for Quantum Organic Chemistry (GQOC) is concerned with the application of state-of-the-art theoretical approaches to important problems in organic chemistry and biochemistry. Particular focus is devoted to understanding of the structure and function of proteins and the properties and design of functional molecules such as (super) acids and bases.

Ivan Halasz, of the RBI Laboratory for the synthesis of new materials, has discovered, in collaboration with an international team of scientists, a brand new, innovative and ecological method for investigating chemical reactions that could improve understanding of the chemical processes essential for the pharmaceutical, chemical and metallurgical industries and open new opportunities in the field of 'green chemistry', as well as the creation of new environmentally friendly chemical products. Bulk solvents which are omnipresent in the chemical industry pose a serious threat to human health and the environment. As a result, there is a growing interest in avoiding their use by relying on 'mechanochemistry' as an energy-efficient alternative that uses high-frequency milling to drive reactions. However, due to intense impact of steel balls in rapidly moving jars the underlying chemistry is difficult to observe. Scientists have now for the first time studied a milling reaction in real time, using highly penetrating X-rays to observe the surprisingly rapid transformations as the mill mixed, ground, and transformed simple ingredients into a complex product. This research, reported Dec. 2 in Nature Chemistry (IF 20), promises to advance scientists' understanding of processes central to the pharmaceutical, metallurgical, cement and mineral industries. The research results are, therefore, great news for the environment, industry and consumers. The international team of scientists from the University of

Cambridge (UK), Max-Planck-Institute for Solid State Research in Stuttgart (Germany) and the European Synchrotron Radiation Facility (ESRF) in Grenoble (France) was led by Tomislav Friščić of McGill University (Canada) and Ivan Halasz from RBI.

Krešimir Jakovčić, Milica Krčmar, Biljana Lakić, and Ante Ljubičić, of the Division of Experimental Physics (Laboratory for Electromagnetic and Weak Interactions), in cooperation with colleagues from the international collaboration of CERN Axion Solar Telescope (CAST), published a paper entitled "Search for Sub-eV Mass Solar Axions by the CERN Axion Solar Telescope with He-3 Buffer Gas", an Editors' Suggestion in the journal Physical Review Letters. The paper presents the latest results in the search for solar axions being conducted in the CAST experiment since 2003. Axions are hypothetical particles, originally proposed as a solution to the significant CP problem in quantum chromodynamics, and are also candidates for cosmological dark matter. The search for them has lasted about thirty years and a signal of their existence has yet to be found.

In 2012 it was confirmed by the European Centre for Nuclear Research (CERN) that a new subatomic particle has been detected with the characteristics of the Higgs boson, popularly known as the "God particle." Scientists working on the projects CMS and ATLAS presented the results of their research, which confirmed that the new particle decays into two photons, indicating that it is a boson in the mass region around 125-126 GeV, the heaviest boson ever found. Participants in the CMS experiment included two scientists from the Ruđer Bošković Institute (RBI), Vuko Brigljević and Krešo Kadija, together with the research assistants Senka Đurić, Srećko Morović and Jelena Luetić. The RBI scientists in the CMS collaboration have the leading role in measuring the processes in which pairs of boson particles are formed. Such processes represent significant background in the search for the Higgs boson, the precise measurement of which is an important factor. The research assistants Senka Đurić and Srećko Morović are currently completing their doctorates on the first measurements of such processes, while Vuko Brigljević is the leader of the CMS group that is responsible for such measurements.

The book "Microwave Assisted Cycloaddition Reactions" by Davor Margetić, a member of the Laboratory for Physical-Organic Chemistry in the Division of Organic Chemistry and Biochemistry of the Ruđer Bošković Institute, was published as part of the series Chemical Engineering Methods and Technology by the New York publishing house of Nova Science Publishers, Inc., New York. The book demonstrates the importance of using microwave assisted organic synthesis as a new experimental technique, which makes modern organic synthesis more ecologically acceptable due to significantly enhanced reaction efficiency, lower energy consumption and a reduction in toxic organic wastes.

Projects and other revenue

In 2012, RBI had 128 projects in basic research funded by the Ministry of Science Education and Sport. The Institute is involved with almost 100 international projects (including 18 FP7, 2 IPA, 7 IAEA, 1 NATO, 24 COST, 1 SCOPES, and 59 bilateral projects), as well as around 50 domestic competitive projects and applied and technological contracts (including 9 HRZZ, 1 HIT and 2 BICRO). In addition to the summary in Table 3, the total financial value of these projects can be seen in Table 4, as well as the funding trends since 2007. The details of the projects involving RBI scientists in 2012 are to be found in the subsequent sections of this report. Nevertheless, we present here two projects in order to convey a general impression of the kind of projects being implemented at the Institute.

Scientists at the RBI Centre for Marine Research (CMR) in Rovinj led by Dr. Renato Batel are a part of the EU FP7 consortium BlueGenics worth 6 million euros. This collaborative project aims at investigating bioactive compounds and developing sustain-

able production of bioactive molecules existing both in moderate, as well as unexploited extreme environments, eventually leading to the development of innovative marine biodiscovery pipelines for novel industrial products. The aim of this industry-driven integrating project is to combine the knowledge in marine genomics, chemogenetics and advanced chemistry to produce recombinant prepared novel secondary metabolite (lead) compounds and their analogues, as well as pharmacologically active peptides, and to bring them up to pre-clinical, and hopefully also to clinical studies. This ambitious approach is based on breakthrough discoveries and the results of previous successful EU projects of members of the applying consortium, including European leaders in marine (sponge) genomics, metagenomics (polyketide synthase clusters), combinatorial biosynthesis and marine natural product chemistry/structure elucidation. The molecular-biology-based strategies developed in this project for a sustainable exploitation of aquatic molecular biodiversity will further strengthen the international position and effectiveness of European (SME-based) blue biotechnology industry.

PROJECT	TOTAL NO.	FIELD OF RESEARCH
FP7	18	COMPUTER SCIENCES, EXPERIMENTAL PHYSICS, NANOMATERIALS, ENVIRONMENT
NATO	1	BIOMEDICINE AND MOLECULAR BIO SCIENCES
IAEA	7	EXPERIMENTAL PHYSICS
COST	24	BIOMEDICINE AND MOLECULAR BIO SCIENCES, NANO SCIENCES, CHEMISTRY, MOLECULAR SCIENCES AND TECHNOLOGY, ECOLOGY, FOOD AND AGRICULTURE, SOCIETY, CULTURE AND HEALTH
IPA	2	TECHNOLOGY TRANSFER, TRANSLATIONAL MEDICINE
SCOPES	1+1	ENVIROMENT, EXPERIMENTAL PHYSICS

Table 3. A summary of international project success in 2012

RBI scientists in the Division for Marine and Environmental Research in Zagreb and the Centre for Marine Research in Rovinj, led by Daniel Lyons, are part of the recently launched four-year project, operating under the European Commission's 7th Framework Program SMART-NANO, worth 3.5 million euros. In response to the increasing need for the detection and analysis of nanoparticles, European industry and academics have launched the EU-funded SMART-NANO project. The aim of this research and development effort, which brings together 3 non-profit and 5 SME partners from 7 countries, is to develop an innovative, cost-effective technology platform that provides a total solution 'from-sample-to-result' for the detection, identification, and measurement of engineered nanoparticles in a wide range of matrices. The consortium's principal purpose of developing a technology platform for the measurement of engineered nanoparticles (ENPs) could provide the key tool in assessing the fate and potential safety risks of ENPs for example in cosmetic products. The outcome of the project will be a miniaturized, modular, cartridge-based technology platform integrating all analytical steps needed for separation, detection, and quantification of ENPs in complex matrices. Parallel to the development of the technology platform, analytical methods and protocols will be developed and tested in the field, resulting in a ready-to-use cartridges for immediate, widespread use in real-life applications.

Table 4. also shows that the largest non-competitive source of revenue continues to be derived from the Ministry of Science, Education and Sports, which directly contributed almost € 22 M in 2012. A significant part of this revenue is dedicated to staff salaries (ca. 75%), while the remainder is principally related to various running costs. This so-called block grant was reduced in 2010. The total RBI revenue was reduced by almost € 3 M in comparison to 2010.

According to the latest financial statements for the year 2012, the Institute is funded, approximately as follows: 90% from the State

REVENUE	2007	%	2008	%	2009	%	2010	%	2011	%	2012	%
Funding from the Ministry of Science, Education and Sports (MSES)	23,770.52	83.61%	25,755.01	86.37%	24,030.18	83.82%	23,372.73	81.61%	21,628.32	87.40%	21,602.56	90.16%
National project funding (Croatian Science Foundation, Croatian Institute of Technology, etc.)	1,017.19	3.58%	487.601	1.64%	345.916	1.21%	1,365.29	4.77%	941.694	3.81%	452.728	1.89%
International project funding (FP, NATO, IAEA, etc.)	1,377.93	4.85%	910.305	3.05%	1,575.53	5.50%	1,780.55	6.22%	1,042.51	4.21%	526.51	2.20%
Commercial contracts	1,999.84	7.03%	2,449.66	8.22%	2,416.48	8.43%	1,873.09	6.54%	1,116.29	4.51%	1,372.34	5.76%
Donations and other funding	264.046	0.93%	216.622	0.73%	300.392	1.05%	246.147	0.86%	16.619	0.07%	6.224	0,026&
TOTAL	**28,429.53**	**100%**	**29,819.20**	**100%**	**28,668.50**	**100%**	**28,637.81**	**100%**	**24,745.43**	**100%**	**23,960.36**	**100%**

Table 4. RBI Revenue from 2007-2012 (€)

Budget of the Republic of Croatia through the Ministry of Science, Education and Sports, 6% through cooperation with businesses, mainly through services and several joint research projects, 3% through aid from abroad and international organizations (EU projects) and 2% from subjects within the general budget, including the Croatian Science Foundation (NZZ), and the Instrument for Pre-Accession Assistance (IPA).

Organization of international conferences and outreach activities

As in previous years, the RBI continued to support the organization of numerous international and domestic conferences, some particular examples of which are mentioned below.

As part of International Hands-on Particle Physics Masterclasses, in March, the RBI was visited by a group of 40 high school students who had the opportunity to analyse real data from the Large Hadron Collider (LHC), the largest and highest-energy particle accelerator in the world, located at CERN. In addition to visiting the RBI, the students also visited the Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, University of Split. High school students from around the world spent one day working as scientists from February to March. Their day as researchers began with a lecture on the research program at CERN and a simplified method for analysing the events of proton collisions accelerated in the LHC. The lecture was followed by data analysis. The research day concluded with a video link-up with CERN and other institutions, when the results of their analyses were compared and discussed.

The largest vacuum-related meeting in Europe in 2012 - a quadruple JVC-14 / EVC-12 / AMDVG-11 / CroSloVM-19 meeting was organized in June in Dubrovnik, under the auspices of Croatian President Ivo Josipović. The four events were merged together into a single conference, with a unified program and lectures, and one overriding registration. Dubrovnik, a traditional meeting place for international cooperation offered an excellent and stimulating environment for the conference of high scientific merit which attracted participants from all over Europe. World-renowned scientists presented plenary lectures, a number of internationally acknowledged researchers held invited speeches, and numerous oral and poster contributions were provided as insight into state-of-the-art of science and technology in the fields powerfully affecting modern society.

The second session of the Adriatic School on Nanoscience ASON-2 was held in September in Dubrovnik, which gathered fifteen world-renowned speakers, including Nobel Laureate Professor Harold Kroto and fifty doctoral and postdoctoral students from Europe and Asia.

Awards and recognition

The achievements of RBI scientists in 2012 were also recognized through numerous awards.

Former RBI scientist academic Vitomir Šunjić and RBI research scientist Tomislav Domazet-Lošo received State Awards for Science. The Lifetime Achievement Award was

presented to Vitomir Šunjić in recognition of his overall scientific research and exceptional contribution to the expansion of scientific knowledge and the application of results in the field of the natural sciences. Tomislav Domazet-Lošo was presented the Annual State Science Award for scientific achievements in the area of the natural sciences.

Tomislav Domazet-Lošo was also awarded the Order of the Croatian Morning Star for Science with the Image of Ruđer Bošković for outstanding contributions to science and its promotion in the Republic of Croatia and the world. Dr. Domazet-Lošo is a distinguished young scientist who, with the discovery of the method of genomic phylostratigraphy, has provided strong evidence supporting the theory of evolution. His research demonstrated for the first time that even simple organisms can have tumours, which is of great significance to medicine.

RBI Scientist Emeritus Ivo Šlaus was elected President of the World Academy of Art & Science. For the first time in history, the headquarters of the WAAS is located in the Republic of Croatia, at the Ruđer Bošković Institute. With the motto "Leadership in thoughts that leads to action," the WAAS provides eminent intellectuals with a politically independent forum for the discussion of vital problems of humanity and promoting science for the general good of society. The main focus of the WAAS is to improve human capital while cooperating with a number of international organizations, such as the Club of Rome, Pugwash movement, the European Leadership Network and All European Academies (ALLEA). The World Academy of Art and Science was established at the initiative of Albert Einstein, Bertrand Russell, Robert Oppenheimer, Harold Urey, Pierre Auger, Harold Lasswell, Francis Perrin, Joseph Rotblat and John Boyd Orr, a Nobel laureate who became its first president in 1960. Today, the WAAS has over 600 members from 86 countries throughout the world.

Nela Pivac, Senior Scientist at the Ruđer Bošković Institute was presented with the Ante Šercer Award by the Academy of Medical Sciences. The Award was presented in recognition of the best scientific paper published in the year 2011: 'Brain derived neurotrophic factor Val66Met polymorphism and psychotic symptoms in Alzheimer's disease' which was published in Progress in Neuro-Psychopharmacology & Biological Psychiatry. The paper shows for the first time that distribution of the BDNF Val66Met genotypes differed significantly between male and female Azheimer's patients with or without psychotic symptoms. The additional special value of this work lies in its multidisciplinary approach since it brought together scientists and clinicians from medical institutions, researchers from the University Hospital Centre in Zagreb, the University of Zagreb School of Medicine, the Institute for Medical Research and Occupational Health in Zagreb, the Psychiatric Hospitals 'Sveti Ivan' and Vrapče as well as the Ruđer Bošković Institute.

Two RBI research assistants Martina Malnar of the Laboratory for Molecular Neuropharmacology and Galja Pletikapić of the Laboratory for Bioelectrochemistry and Surface Imaging received Women in Science Fellowships for 2012. L'Oreal Adria and the Croatian Commission for UNESCO annually rewards the most successful young female scientists in the natural sciences and interdisciplinary fields, who are in the final stage of preparing their doctoral dissertations.

Following several notable successes by the promising young RBI scientist Robert Vianello, Ph.D., his FP7 project Computational Studies of Proton Dynamics in Hydrogen Bonded Systems and Enzymes (CoSProDyn) was presented as a success story of the European Commission. The project was featured among 23 selected individual Marie Curie Fellowship recipients in a publication issued in Brussels entitled EU FP7 People Specific Programme Success Stories Booklet, in which a total of 45 successful Marie Curie projects throughout Europe were presented.

Education

Although the RBI does not have the legal possibility of independently conducting doctoral studies, it has initiated a large number of doctoral and specialist studies in cooperation with universities in Croatia. Furthermore, on the basis of agreements with various universities in Croatia, RBI scientists actively participate in teaching at the undergraduate level.

By far the strongest collaboration is with the University of Zagreb, with which a formal cooperation agreement was signed in 2007. Most of this cooperation takes place at the Faculties of Science, Electrical Engineering and Computing, Agriculture and Medicine. Together with the Josip Juraj Strossmayer University in Osijek, in 2002 the RBI launched the interdisciplinary postgraduate study Nature and Environmental Protection, which has operated as doctoral and specialist studies since 2008. Annually, an average of 10 students are enrolled in the doctoral studies and 15 in the specialist studies.

In 2006, a joint postgraduate interdisciplinary doctoral program in Molecular Biosciences was launched by the RBI in collaboration with the Josip Juraj Strossmayer University in Osijek and the University of Dubrovnik, in which an average of 40 students enrol each year. In collaboration with the Universities of Split, Dubrovnik and Zadar, in 2006 the RBI inaugurated Postgraduate Doctoral Studies in the Biology of Neoplasms, and on the basis of an agreement on cooperation with the Faculty of Medicine, University of Zagreb,

	Academic year				
	2008/09	**2009/10**	**2010/11**	**2011/12**	**2012/13**
Number of undergraduate courses	315	378	373	382	403
Number of graduate courses	166	179	174	174	179
Number of postgraduate (PhD) courses	33	48	40	42	41
Supervision of graduate theses	203	228	220	223	223
Supervision of postgraduate (PhD) programmes (number of school hours)	11995	14372	13993	13620	15525
Number of specialist postgraduate programme courses	275	335	323	339	353
Organizing and holding professional program courses	157	172	168	170	174
Participation of research assistants in teaching (number of school hours)	5408	6478	6302	6252	6739
Number of undergraduate courses	8	10	10	9	16
Number of graduate courses	384	459	617	523	723
Number of postgraduate (PhD) courses	42	65	77	73	76
Supervision of graduate theses	37	53	53	58	58
Supervision of postgraduate (PhD) programmes	198	216	198	208	213
Number of specialist postgraduate programme courses	3	4	4	6	7
Organizing and holding professional program courses	5	1	0	0	5
Participation of research assistants in teaching (number of courses)	4	5	4	3	4

Table 5. Overview of the teaching activities of RBI staff in 2012.

the RBI participates in Postgraduate Studies in Biomedicine and Health, and in Doctoral Studies in Neurosciences. Based on an agreement for cooperation with the Faculty of Science of the University of Zagreb, the Institute of Marine and Coastal Research of the University of Dubrovnik, and the Institute of Oceanography and Fisheries in Split, the Ruđer Bošković Institute has participated in the joint Interdisciplinary Postgraduate University Studies in Oceanology since 2006. In the year 2010, the RBI launched joint Doctoral Studies in the Chemistry of the Mediterranean Environment, as well as in Biophysics with the University of Split. Pursuant to a partnership agreement signed in 2007 with the Juraj Dobrila University of Pula, the Ruđer Bošković Institute organizes university Undergraduate Studies in Marine Sciences, and RBI scientists teach a total of 72 courses in this program. The same year saw an agreement signed with the

University of Rijeka for launching Undergraduate, Graduate and Doctoral studies in Medicinal Chemistry. The first part of these joint studies, the Undergraduate Studies in Biotechnology and the Study of Medications at the Department of Biotechnology, University of Rijeka, had 40 and 54 enrolled students, respectively during the 2009/2010 academic year. It should be particularly noted that during the recent past, research assistants of the Institute were included in teaching, especially in conducting practical and laboratory exercises and seminars. From 2008 to 2012, the

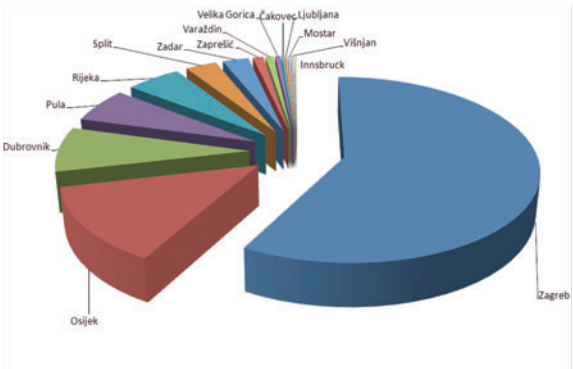


Figure 4. The distribution of the RBI courses by the location of the relevant hosting institution

number of courses per scientist was 1.26, which indicates a high rate of participation by RBI scientists in university study programs. Details can be seen in table 5 as well as figures 4 and 5.

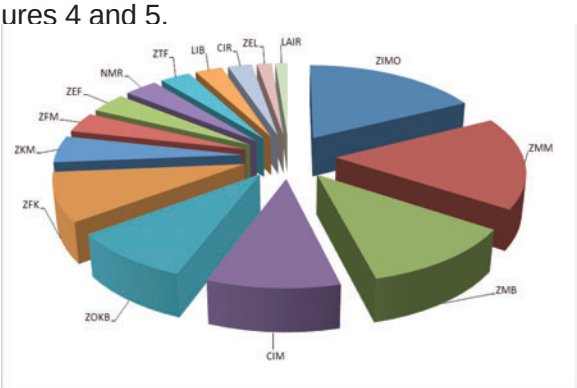


Figure 5. The distribution of the RBI courses by RBI Division

Intellectual Property

Apart from fundamental research and education, the activities of the RBI also result in various forms of intellectual creations. One important aspect of the RBI's mission is the protection of intellectual property and its commercialization. In this context, various specific activities have been initiated and realized over the last few years. As a subsidiary, the Ruđer Bošković Institute established Ruđer Innovations Ltd., a company specializing in the commercialization of innovations and technology transfer. The intellectual property portfolio of Ruđer Innovations includes innovations protected by patents or patent applications in various fields of science that have commercial potential. In 2012 the United States Patent Office accepted three patent applications from the RBI scientists.

U.S. Patent No. US 8, 217, 022 B2, entitled: Analogues of 1, 3-bis(4-nitrophenyl) triazenes, their pharmaceutically acceptable salts and N-acyl derivatives for tumour treatment was issued to Maja Osmak, Polanc Slovenko, Tamara Čimbora-Zovko, Anamaria Brozović, Marjan Kočevar, Vita Majce, Branko Alić. The present patent gives the 1, 3-bis (4-nitrophenyl) triazenes, their pharmaceuti-

cal acceptable salts and N-acyl derivatives that inhibit the cell division and they could be potentially used for cancer treatment. The selected representatives from this new group of compounds are highly cytotoxic to tumour cells and their drug-resistant subline, but less cytotoxic to normal cells.

U.S. Patent No: US 8, 165, 373, entitled: Method of and system for blind extraction of more pure components than mixtures in 1D and 2D NMR spectroscopy and mass spectrometry combining sparse component analysis and single component points was issued to Ivica Kopriva and Ivanka Jerić. A computer-implemented data processing system for blind extraction of more pure components than mixtures recorded in 1D or 2D NMR spectroscopy and mass spectrometry. Sparse component analysis is combined with single component points (SCPs) to blind decomposition of mixtures data X into pure components S and concentration matrix A, whereas the number of pure components S is greater than number of mixtures X. NMR mixtures are transformed into wavelet domain, where pure components are sparser than in time domain and where SCPs are detected. Mass spectrometry (MS) mixtures are extended to analytical continuation in order to detect SCPs. SCPs are used to estimate number of pure components and concentration matrix. Pure components are estimated in frequency domain (NMR data) or m/z domain (MS data) by means of constrained convex programming methods. Estimated pure components are ranked using negentropy-based criterion.

U.S. Patent No: US 8, 224, 427, entitled: Method for real time tumour visualisation and demarcation by means of photodynamic diagnosis was issued to Ivica Kopriva. Patent is related to the field of photodynamic therapy and photodiagnosis. Specifically, a new algorithm is presented for the visualisation and spatial demarcation of various types of tumours and unhealthy tissue through unsupervised segmentation of the fluorescent multispectral image. An image is acquired through recording of the emission of the tissue illuminated by the light that induces fluorescence in the tumour. For this purpose, tissue is treated by photo sensitizer. The algorithm for real time visualisation and spatial demarcation of the tumour, by means of the analysis of fluorescent image, consists of: the recording of the fluorescent image that represents a linear combination of the unknown classes S by multispectral camera, transformation of the fluorescent multispectral image into new multispectral image, applying nonlinear dimensionality expansion, linear transformation of the multispectral image with extended dimensionality, independent component analysis of the innovation representations of the multispectral image that is the result of the transformation of the fluorescent image and the multispectral image, extraction of the tumour map or class of interest in accordance with the chosen criterion and visualisation of tumour on the monitor.

Theoretical Physics Division

http://www.irb.hr/en/str/ztf

DIVISIONAL ORGANIZATION

Head: Željko Crljen

The Theoretical Physics Division (ZTF) consists of the following laboratories:

- Solid State Physics Group, Radovan Brako (to July 27, 2012); Damir Šokčević
- Particle Physics and Cosmology Group, Neven Bilić
- Theoretical and Mathematical Physics Group, Stjepan Meljanac

OVERVIEW OF THE DIVISION

Research activities in the Theoretical Physics Division are focused on broad areas of theoretical physics: from particle physics, gravity and mathematical physics to condensed matter physics.

The research in particle physics involves investigations in particle and collider physics, perturbative quantum chromodynamics and particle cosmology. The non-commutative spaces and quantum field theory and symmetry are also in the core of our interest. Research thrusts in condensed matter physics focus on electronic and magnetic properties of nanoscale systems including spin-dependent transport and on the statistical physics of non-equilibrium phenomena and dynamical complex systems.

The members of the division are engaged in a multitude of activities reaching far beyond the boundaries of the division through international collaborations and projects, as well as through their involvement in lecturing at universities in Zagreb and in Split.

The division is currently undergoing a partial generational change. With our newest members we have a strong commitment to continuing with excellence in research and international scientific exchange and collaboration.

TOP ACHIEVEMENTS

Kappa-deformation of phase space; generalized Poincaré algebras and R-matrix

Coalgebras for the generalized Poincaré algebras and deformed phase space have been constructed and the exact universal R-matrix was found. It was also shown that in the case of kappa-Poincaré algebra this R-matrix can be expressed in terms of Poincaré generators, implying that the many particle states of identical particles can be introduced in a kappa-covariant way (Meljanac et al., 2012).

Geometric origin of scaling in large traffic networks

Large scale traffic networks are an indispensable part of contemporary human mobility and international trade. Different empirical studies point to the universal character of some of the exponents measured in such networks. A simple robust model was developed which exhibits the observed power laws and relates exponents to the dimensionality of 2D space in which traffic networks are embedded. The model was studied both analytically and in simulations and the conditions which result with previously reported exponents are clearly explained (Popović et al., 2012).

Discerning new physics in top-antitop production at hadron colliders

Several top spin observables and the recent top spin correlation measurement by ATLAS is used to consider the consistency of the simplified single-resonance models and to provide a significant constraint on possible explanations of the Tevatron forward-backward asymmetry anomaly. It was shown that future precise measurements of top spin correlations and especially top polarization could differentiate between scalar t-channel models, while they are less sensitive to pure s-channel contributions (Fajfer et. al., 2012).

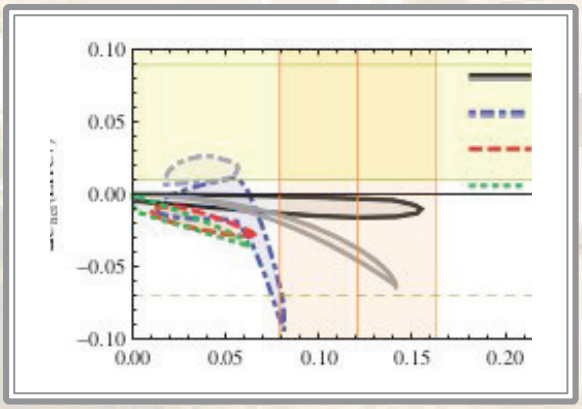


Fig.1. Correlations between various New Physics contributions to the inclusive forward-backward asymmetry at the Tevatron and to the shift of top-antitop spin observable C from corresponding Standard Model values at the 7 TeV LHC. The present experimental results (68% C.L. regions) are shaded in horizontal and vertical bands.

Neutrino propagation in inocommutative spacetimes

The closed form of one-loop θ-exact quantum corrections to the neutrino propagator are computed in noncommutative $U_*(1)$ gauge-theory based on Seiberg-Witten maps. Non-trivial modifications to the neutrino dispersion relations which are asymptotically independent of the scale of noncommutativity at both the low and high energy limits was found for certain unitarity-preserving θ values which allow the cancellation of UV divergence and UV/IR mixing contributions. Effects of Seiberg-Witten map freedom on neutrino propagation is also demonstrated (Horvat et al., 2012).

Geodesic equation in k-Minkowski spacetime

Effects of kappa-deformations on the motion of a particle in curved spacetime is analyzed. The main difference between the commutative and deformed case is that we have an “extra” force, i.e. drag that acts on the particle when moving in a kappa-deformed curved spacetime (Harikumar et al., 2012).

The scale-setting for the effective action of gravity with scale dependent parameters

In effective theories of gravity with scale-dependent parameters the procedure of scale-setting at the level of the action is elaborated. We demonstrate how the scale-setting procedure may lead to an exponentially suppressed effective cosmological constant or to terms in the effective action with inverse powers of the Ricci scalar R. It was shown that the scale-setting procedure leads to a universal form of the effective

gravitational action quadratic in R close to the non-gausssian fixed point, even for arbitrary truncations polynomial in R (Domazet and Štefančić, 2012).

Rationale for switching to nonlocal functionals in density functional theory

The absence of van der Waals interactions in common density functional theory implementations has been a big hurdle in tackling some interesting systems - such as soft matter, organic molecules on metal surfaces etc. Since 2004 the first really nonlocal correlation functional appeared (vdW-DF) which enabled the correct treatment of such systems. However, the impact of this functional appeared to be much larger - somewhat unexpectedly even the strongly chemisorbed systems experienced a change in result when a nonlocal functional was used (Lazić et al., 2012).

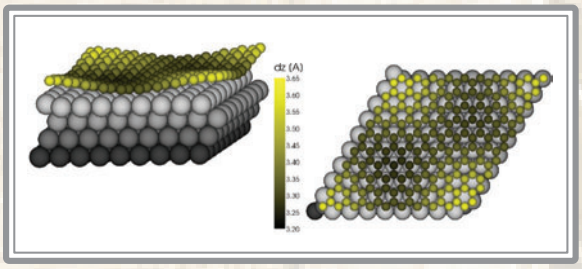


Fig.2. Moiré structure of 10x10 graphene on a 9x9 iridium surface. Left: top view, dz is the distance in Å from the topmost iridium layer. Right: side view, where for reasons of clarity the corrugation is magnified by a factor of five.

Analogue surface gravity near the QCD chiral phase transition

The QCD chiral phase transition in an expanding chiral fluid was studied using the formalism of relativistic acoustic geometry. The dynamics of pions below the critical temperature is described by the equation of motion for a massless scalar field propagating in curved spacetime similar to an open FRW universe. If the analog apparent horizon forms close to the critical temperature the analogue Hawking temperature is comparable with the background fluid temperature (Bilić and Tolić, 2012).

EDUCATION

In 2012, the members of the Division continued to be involved in teaching of undergraduate and graduate courses mostly at the University of Zagreb (Faculty of Science, School of Economics and Management) and the University of Split (Faculty of Science, Faculty of Civil Engineering and Architecture). A number of students completed their B. Sc. and M. Sc. theses.

AWARDS

Stjepan Meljanac, Hrvoje Štefančić, Marko Popović, Anđelo Samsarov and Vinko Zlatić received the RBI Director's Award for Scientific Excelence in 2012.

PROJECTS

Programs supported by the Ministry of Science, Education and Sport

1. Surfaces and nanostructures: Theoretical approaches and numerical calculations, Radovan Brako (to July 12, 2012); Damir Šokčević
2. Electronic properties of hybrid nanostructures, Željko Crljen
3. Fundamental interactions in elementary particle physics and cosmology, Neven Bilić
4. Quantum field theory, noncommutative spaces and symmetries, Stjepan Meljanac

Research, developmental and international project

1. Geometry and quantum field from noncommutative landscape, Larisa Jonke (Croatian-

Austrian bilateral project), MSES, EUR 2.700
2. Integrable systems and noncommutative structures, Stjepan Meljanac (Croatian-French bilateral project in the program "COGITO"), MSES, EUR 4.300
3. Forecasting Financial Crises, Vinko Zlatić (EU FP7-ICT-255987 – FOC-II Project), EUR 170.560

SELECTED INVITED LECTURES

1. Trampetić J: High energy cosmic rays experiment inspired by noncommutative quantum field theory, The fifth Petrov International Symposium on High Energy Physics, Cosmology and Gravity, Kyiv, Ukraine, April 29 – May 5, 2012.
2. Nikolić H : Solipsistic hidden variables, Quantum 2012: Advances in Foundations of Quantum Mechanics and Quantum Information with Atoms and Photons, Torino, Italy, May 21-25, 2012.
3. Melić B: Discerning a new physics in ttbar production from spin observables, PASCOS2012 - 18th International Symposium on Particles Strings and Cosmology, Merida, Mexico, June 3-8, 2012.
4. Bilić N: Accelerated expansion of the Universe and dark energy, 27th Summer School in Physics: The Universe and Life in Physics, Mali Lošinj, Croatia, June 17-23, 2012.
5. Škoda Z: Model theory and noncommutative geometry, Encuentro de Matematicas 2012, Bogota, Colombia, July 24-26, 2012.
6. Bilić, N: Effective vacuum energy of the supersymmetric field in curved background, IRGAC-2012 – International Conference on Quantum Theories and Renormalization Group in Gravity and Cosmology, Rio de Janeiro, Brazil, July 29 – August 3, 2012.
7. Škoda Z: Hopf torsors over corings, ESF Exploratory workshop „Interfaces on Noncommutative Geometry with the Representation Theory of Hopf Algebras and Artin Algebras", Istanbul, Turkey, August 7-10, 2012.
8. Lazić P: The role of the nonlocal correlation in surface adsorption, CECAM/Psi-k Workshop 2012 - Functional Molecules on Surfaces: New Building Blocks for Nano-spintronics, Bonn, Germany, October 2-4, 2012.

SELECTED ORGANIZED CONFERENCES

1. Bayrischzell Workshop 2012 - Noncommutativity and Physics: Spacetime Quantum Geometry, Bayrischzell, Germany, May 25-28, 2012 (Josip Trampetić, member of the Organizing Committee).
2. ASON-2 - 2nd Adriatic School of Nanoscience, Dubrovnik, Croatia, September 2-7, 2012 (Predrag Lazić, member of the Program Committee).

SELECTED PUBLICATIONS

1. Popović M, Štefančić H, Zlatić, V. Geometric origin of scaling in large traffic networks, *Phys Rev Lett* **109** (2012) 208701.
2. Meljanac S, Samsarov A, Štrajn R. Kappa-deformation of phase space; generalized Poincare algebras and R-matrix. *J High Energy Phys* **08** (2012) 127.
3. Fajfer S, Kamenik J F, Melić B. Discerning New Physics in Top-Antitop Production using Top Spin Observables at Hadron Colliders. *J High Energy Phys* **2012** (2012) 114.
4. Horvat R, Ilakovac A, Schupp P, Trampetić J, You J. Neutrino propagation in noncommutative spacetimes. *J High Energy Phys* **12** (2012) 108-1.
5. Chatzistavrakidis A, Jonke L. Matrix theory compactifications on twisted tori. *Phys Rev D* **85** (2012) 1.
6. Dimitrijević M, Radovanović V, Štefančić H. AdS-inspired noncommutative gravity on the Moyal plane. *Phys Rev D* **86** (2012) 105041-1.
7. Harikumar E, Jurić T, Meljanac S. Geodesic equation in k-Minkowski spacetime. *Phys Rev D* **86** (2012) 45002.
8. Bilić N, Tolić D. Analogue surface gravity near the QCD chiral phase transition. *Phys Lett B* **718** (2012) 223.

9. Horvat R, Ilakovac A, Schupp P, Trampetić J, You J. Yukawa couplings and seesaw neutrino masses in noncommutative gauge theory. *Phys Lett B* **715** (2012) 340.
10. Bilić N, Domazet S, Guberina B. Vacuum fluctuations of the supersymmetric field in curved background. *Phys Lett B* **707** (2012) 221.
11. Kovačević D, Meljanac S, Pachol A, Štrajn R. Generalized Poincaré algebras, Hopf algebras and kappa-Minkowki spacetime. *Phys Lett B* **711** (2012) 122.
12. Lenac Z, Crljen Ž. Wigner lattice in between two dielectric slabs: Image potential and Casimir effect. *Phys Rev A* **86** (2012) 022524-1.
13. Lazić P, Atodiresei N, Caciuc V, Brako R, Gumhalter B, Blugel S. Rationale for switching to nonlocal functionals in density functional theory, *J Phys Condens Matter* **24** (2012) 424215.
14. Domazet S, Štefančić H. Renormalization group scale-setting from the action—a road to modified gravity theories. *Classical Quant Grav* **29** (2012) 23.

Chapters in books

1. Nikolić H. Relativistic Quantum Mechanics and Quantum Field Theory. Applied Bohmian Mechanics: From Nanoscale Systems to Cosmology / Oriols, Xavier; Mompart, Jordi (ed). Singapore: Pan Stanford Publishing, 2012. pp 455-505.

Division of Experimental Physics

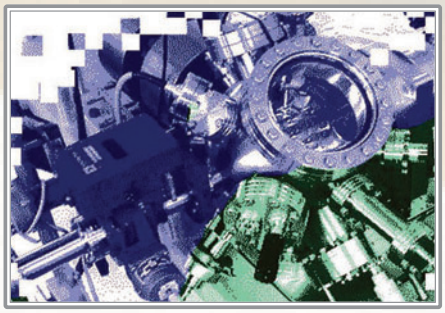
http://www.irb.hr/en/str/zef

DIVISIONAL ORGANIZATION

Head: Tome Antičić (until August 19, 2012), Milko Jakšić (from August 20, 2012 and November 8, 2012)

The Division of Experimental Physics consists of the following laboratories:

- Laboratory for hadron physics, Ivan Supek
- Laboratory for nuclear physics, Zoran Basrak
- Laboratory for astroparticle physics, Raul Horvat
- Laboratory for electromagnetic and weak interactions, Milica Krčmar
- Laboratory for ion beam interactions, Milko Jakšić
- Laboratory for measurement of low-level activities, Nada Horvatinčić
- Laboratory for high energy physics, Krešo Kadija
- Laboratory for nuclear analytical methods, Jasmina Obhođaš
- Group for hadronic spectroscopy, Alfred Švarc



OVERVIEW OF THE DIVISION

The core activities of the Division of Experimental Physics (DEP) involve experimental ion beam, nuclear, particle and astroparticle physics, as well as related radiation applications. The division staff is involved in international collaborations at experimental facilities abroad and in Croatia and maintains a strong performance in both basic and applied physics research. A large fraction of its financing comes from external sources, which was used, among other things, to significantly enhance its experimental capabilities.

The main strategic objectives of the DEP for the next five years are briefly:

- A significantly enlarged experimental contribution to top level, large international physics collaborations, in particularly by enhancing contributions by local experimental work, leading to a much more prominent role in these experiments.
- Increased experimental capabilities and capacities for experiments at the local RBI Tandem accelerator facility.
- Increased utilization of other local experimental capabilities and in particular the Cockcroft Walton accelerator (neutron generator), laboratories for low level radiation measurements and detector testing capabilities using radiation sources and laser light.
- Exploration of application possibilities in interdiscipinary work such as modification and characterisation of advanced materials using ion beams, C-14 dating

using accelerator mass spectrometry, applications of PET isotope imaging capabilities in medicine, employment of radiation techniques in the detection of explosives and interdisciplinary research related to fusion.

- Improved cooperation with Universities, by increasing the role of DEP resources in education, both human and experimental. Search for the best doctoral and postdoctoral candidates as well as funding sources for their education.
- Strengthened partnerships at numerous levels with prominent research institutions across Europe and the wider international community as the basis for enhancing research quality as well as external funding.

TOP ACHIEVEMENTS

Discovery of a new boson at a mass of 125 GeV in the search for the Higgs boson at the LHC

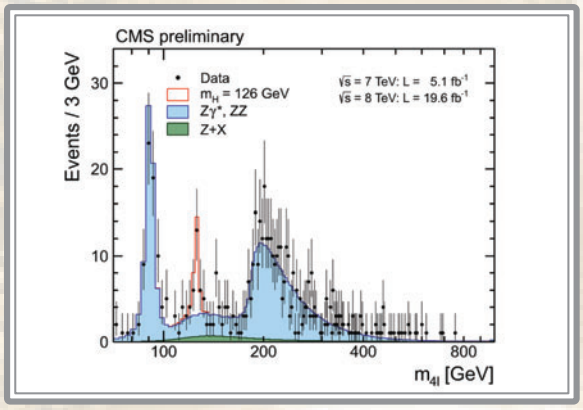


Fig. 1. Distribution of the four-lepton reconstructed mass for pairs of Z bosons based on data collected in 2011 and 2012 by the CMS experiment at the Large Hadron Collider. Evidence for a new boson consistent with the Higgs boson can be seen in the peak around 125 GeV.

The discovery of a new boson consistent with the long sought Higgs boson in the CMS and ATLAS experiments at the LHC in the Summer of 2012 has been one of the most publicised science events in 2012. The RBI group in the CMS Collaboration has continued to play a very active role in the data analysis and running of the CMS detector. The group has held a leadership position in the measurement of diboson processes, which constitute the most important background in the search for the Higgs boson. The group has also actively contributed to the efficient running of the CMS detector in 2012, with a member of our group holding a key responsibility in the online Event Filter processing (Chatrchyan S. et. al., 2012).

Advanced Gamma Tracking Array – AGATA

AGATA is being realized within a European collaboration and is employed in experimental campaigns at radioactive and stable beam facilities in Europe. AGATA, the first complete 4π γ-ray spectrometer built solely from Germanium (Ge) detectors, is based on the novel technique of γ-ray tracking. AGATA is an instrument of major importance for nuclear structure studies at the very limits of nuclear stability, capable of measuring radiation in a very large energy range, with the largest possible efficiency and with a very good spectral response. AGATA (in its full configuration) will be several orders of magnitude more powerful than any current or near-future γ-ray spectrometer, and will be capable of disentangling the structure of exotic nuclei produced with extremely small cross sections in an overwhelming background of ordinary nuclei.

A programme to develop a new generation of position-sensitive high-purity Germanium detectors began in the 5th EU Framework Programme, where a concept for γ-ray tracking was developed. The funding of the AGATA demonstrator, comprising a sub-set of five detector units with full tracking capability, was agreed upon in 2002, and a first physics campaign with the demonstrator was successfully carried out at the Legnaro laboratory, where it was coupled to a PRISMA spectrometer. During this campaign a total

of 20 different physics cases were measured with about 3500 hours of beam-on-target.

The Crystal Ball Spectrometer at MAMI, Mainz

During this year the Crystal Ball Collaboration at the Mainz Microtron (MAMI) successfully continued to use both a transversely and longitudinally polarized target. RBI scientists have significantly contributed to the assembly and running of this new state-of-the–art Frozen Spin Polarized Target. This new target/detector setup enables investigation of many double polarization measurements for the first time. The CB Collaboration has already published more than a dozen publications in high impact journals (Zehr et al., Kashevarov et al., Pheron et al., 2012).

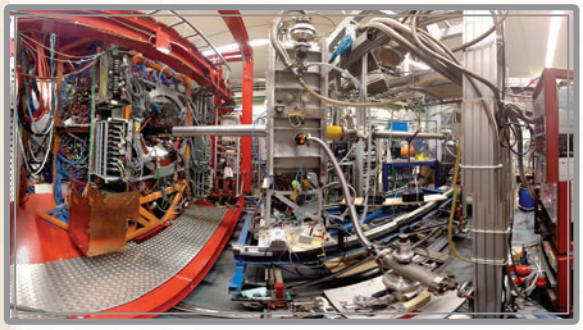


Fig. 2. Frozen Spin Target at MAMI.

Measurement of the neutrino velocity with the OPERA detector in the CNGS beam

At LNGS, the OPERA-RBI group has participated in data collection and analysis of muon neutrino data. An arrival time of CNGS muon neutrinos, with respect to the one computed assuming the speed of light in vacuum, was measured corresponding to a relative difference of the muon neutrino velocity with respect to the speed of light $(v-c)/c=(2.7\pm3.1(\text{stat.})+3.4(\text{sys.})-3.3(\text{sys.}))\times10^{-6}$ (Adam et al., 2012).

Observation of Crab pulsar at the highest energies by MAGIC telescopes

The MAGIC telescopes have been used to observe the pulsar in gamma rays and have detected periodic pulsed emission at energies as high as 400 GeV. This is 50-100 times higher than predicted by current theoretical models. The RBI group, a part of the Croatian MAGIC consortium, has actively contributed to data collection and analysis.

Fig. 3. MAGIC telescopes on the Canary island of La Palma.

A bound on the scale of spacetime noncommutativity

We have made use of a reasonable expectation that thermal epochs in the universe are successfully describable by conventional quantum field theories. After having considered the field-theoretical realization of noncommutative gauge field theories by making use of the specific UV/IR relationship attributive to such an approach, we have shown that an adequate description of the reheating stage after inflation entails a very strong upper bound on the scale of noncommutativity. (Horvat and Trampetić, 2012)

Accelerator provides Trans National Access (TNA) for European scientists

The accelerator facility continued to host numerous international research teams with a total of 107 accelerator days dedicated to experiments proposed by researchers from

abroad. 42 scientists from 15 countries conducted measurements in the fields of nuclear and atomic physics, radiation detector development, material science and environment research. Most of the visits were funded by the FP7 Project SPIRIT where our Institute acted as a provider for Trans National Access (TNA). Within the TNA scheme, scientists from the EU and associated states were granted beam time at the RBI accelerator facility. Other visits were funded through the FP7 project Particle detectors, as well as through several other IAEA and bilateral projects.

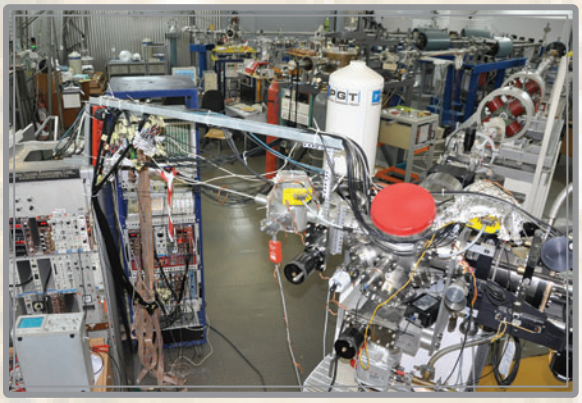


Fig. 4. Experimental hall of the RBI accelerator facility with ion microprobe beam line in front.

Influence of ion beam properties on quantum dot ordering in amorphous matrices

Different ion-beam properties such as ion type, energy and stopping power value were used to study the self-assembly process in $(Ge+SiO_2)/SiO_2$ multilayers. The results show that the most important parameter for structural manipulation with MeV ion beams is the electronic stopping power S_e. Ion velocity was found to be very important in that it determines the efficiency of the energy transfer to the system. A temperature increase in the system caused by ion beam passage was estimated using a thermal spike model and cluster separation distribution (Bogdanović Radović et al., 2012).

Development of diamond detectors

Charge transport properties of diamond detectors and in particular the influence of radiation-induced defects that limit their use in high radiation environments has been the focus of research in several DEP projects. Within the FP7 Particle detectors project, commercially available single crystal CVD diamonds were used to develop complete working detectors along with data acquisition electronics for energy and timing spectroscopy of MeV energy ions. Through a Cooperative Research Project between Japan (JST) and Croatia (MSES) an ion microbeam technology has been used to explore the capabilities of a thin membrane diamond detector that can serve as both a vacuum-air window and an ion transmission detector. Finally, we continued with the development of technology for fabrication of graphitic electrodes by ion beams through a collaboration with the University of Torino.

Plitvice Lakes investigation - environment and climate changes

Carbon isotopes ^{13}C and ^{14}C are good natural tracers for geochemical/carbon exchange processes in the karst environment: atmospheric CO_2 – soil CO_2 – terrestrial plants – DIC in water – aquatic plants - $CaCO_3$ from water (tufa, lake sediment). Anthropogenic impact/increase of ^{14}C activity in the atmosphere caused by thermonuclear bomb-tests in the early 1960s was recorded in the karst environment of the Plitvice Lakes area with different responses depending on carbon exchange processes (Horvatinčić et al., 2012).

NEW EQUIPMENT

Underwater Coastal Sea Surveyor (UNCOSS)

A system using a neutron sensor installed within a Remotely Operated Vehicle (ROV) for underwater inspection has been developed through the UNCOSS FP7 project. The system can inspect objects for the presence of threat materials, such as explosives and chemical agents, by using alpha particle tagged neutrons from a sealed tube d+t neutron generator to produce characteristic gamma rays within the interrogated object. The UNCOSS field test was recorded and shown by EURONEWS. This technique can be further developed for deep sea floor investigations with applications in the interrogation of infrastructure and sunken objects as well as for the observation and research of natural processes (Valković et al., 2012).

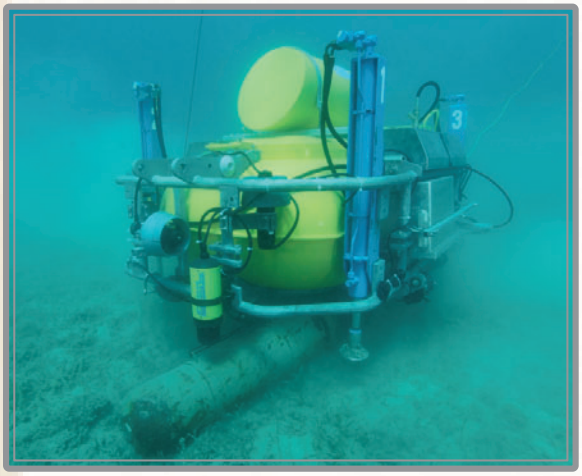


Fig. 5. Underwater inspection of the 20 cm diameter airplane bomb at the depth of 10 meters

Secondary ion mass spectroscopy by MeV ions (MeV SIMS)

A new time of flight spectrometer for secondary ion mass spectrometry has been installed at the heavy ion microprobe facility. This novel analytical technique is based on desorption of molecules and molecular fragments from the sample surface after the impact of a single heavy ion of MeV energy. Due to the possibility of a heavy ion microbeam scanning feature, imaging of molecules (<1000 Da) can be performed with high sensitivity and micrometer spatial resolution. In addition to the University of Kyoto and University of Surrey, the TOF spectrometer at RBI is the third working MeV SIMS system in the world, offering a wide range of application possibilities in particular in biomedical research.

EDUCATION

Members of the Division were involved in lecturing at the undergraduate and graduate level in the Faculty of Science, at the University of Zagreb and University of Rijeka, as well as in joint studies organized by RBI in cooperation with the Universities of Osijek and Dubrovnik. Two students completed their Ph.D. theses and several B.Sc. theses were completed under the leadership of Division staff.

PROJECTS

Projects supported by the Ministry od Sciences, Education and Sports

1. Experimental research of the nucleus: nuclear structures and reactions, Suzana Szilner
2. Ion beam interactions and nanostructures, Milko Jakšić
3. Hadronic physics and QCD, Ivan Supek
4. Heavy-ion physics, Zoran Basrak
5. Massive neutrinos and astro-particles: from particle physics to cosmology, Ante Ljubičić
6. Experimental physics at LHC energies, Krešo Kadija
7. Experiments in quantum communication and quantum information, Mario Stipčević
8. Photon-atom interactions and correlations, Tihomir Surić
9. Natural isotopes in investigation of karst environment and dating, Nada Horvatinčić
10. Development and application of nuclear analytical methods, Jasmina Obhođaš
11. Development of the methods for illicit traffick-

ing control, Dario Matika and Davorin Sudac
12. Hadronic physics between the experiments and QCD models, Alfred Švarc
13. Test of special relativity by the Ives-Stilwell type experiment, Saša Blagus

Research, developmental and international projects

1. Particle Detectors, Tome Antičić project coordinator, FP7-REGPOT project no. 256783.
2. Support of Public and Industrial Research using Ion beam Technology (SPIRIT), Milko Jakšić, FP7-INFRASTRUCTURES project no. 227012.
3. European Nuclear Science and Applications Research (ENSAR), Milko Jakšić, FP7-INFRASTRUCTURES project no 262010.
4. Hadron Physics 3, Ivan Supek, FP7-INFRASTRUCTURES project no 283286
5. Network in solid waste and water treatment between Europe and Mediterranean countries (SOWAEUMED), Bogomil Obelić, FP7 - REGPOT Project
6. Studies, training, socio-economical valorization and management of natural, cultural and monumental property for the promotion of the local societies of Latin America (Argentina, Brazil and Mexico, STRAVAL, Bogomil Obelić, FP7- PEOPLE Project
7. Underwater Costal Sea Surveyor, Jasmina Obhođaš, UNCOSS (FP7-SEC-2007-1)
8. Experimental nuclear physics inputs for thermonuclear runaway, within the collaborative project Physics of compact objects: explosive nucleosynthesis and evolution, Neven Soić, EuroGENESIS programme of the European Science Foundation
9. Exploiting the LHC Potential to build Collaboration in Science and Technology, Vuko Brigljević, SCOPES Institutional Partnership project (RBI, Paul Scherrer Institute and the University of Sarajevo)
10. Enhancement of Ion Beam Analysis Capabilities Using Novel Detection Systems for PIXE, RBS and STIM, IAEA CRP project No 15988, Stjepko Fazinić
11. Radiation hardness of semiconductors and insulators studied by focused ion beam irradiation and IBIC, IAEA CRP project No. 17051, Milko Jakšić
12. Development of a Reference Database for Particle-Induced Gamma-ray Emission (PIGE) Spectroscopy, IAEA CRP project No. 16688, Iva Bogdanović Radović
13. 14C and 137Cs in sediments - comparison of methods and application to recent sediments, bilateral project Croatia – Serbia, Ines Krajcar Bronić
14. Synthesis and modification of titanium based nanocomposite materials by ion and laser beam, bilateral project Croatia – Serbia, Iva Bogdanović Radović
15. Enhanced molecular imaging by focused swift heavy Ions, bilateral project Croatia-Japan, Tonči Tadić
16. Development of high energy ion microbeam technology for novel applications of diamond, bilateral project Croatia-Japan, Milko Jakšić
17. Studies of radiation damage in optical fibers and silicon pin diodes, Technical support agreement with KAERI (Korean Atomic Energy Research Institute), Milko Jakšić
18. Influence of climatic and environmental changes on the processes of biologically induced calcite precipitation in Plitvice Lakes, Project with Plitvice National Park, Nada Horvatinčić
19. Using environmental isotopes for evaluation of streamwater/groundwater interactions in selected aquifers in the Danube basin, project IAEA RER8016, Nada Horvatinčić
20. CERN Axion Solar Telescope (CAST) experiment, Milica Krčmar (International collaboration between RBI and CERN (Switzerland))
21. OPERA collaboration, Ante Ljubičić (International collaboration between RBI, CERN (Switzerland) and LNGS (Gran Sasso, Italy))
22. NA61 Collaboration, Kadija K (International Collaboration between RBI and CERN, Switzerland))
23. NA49 Collaboration, Šuša T (International Collaboration between RBI and CERN, Switzerland))
24. ALICE Collaboration, Antičić T (International Collaboration between RBI and CERN, Switzerland)

25. Pierre Auger Observatory (POA), Kadija, K. (International Collaboration between RBI and POA, Argentina)
26. CMS Collaboration, Kadija K. & Brigljević V. (International Collaboration between RBI and CERN, Switzerland).
27. MAGIC collaboration, RBI membership through Croatian MAGIC consortium

SELECTED INVITED LECTURES

1. Basrak Z: Nuclear stopping at intermediate energies - experiment versus simulation. Workshop on Fluctuations and temporal evolution in heavy-ion collisions, Saclay/Paris, France, May 9–10, 2012.
2. Basrak Z: Scaling of energy deposition in central heavy ion reactions at intermediate energies. 13th International Conference on Nuclear Reaction Mechanisms, Varenna, Italy, June 11-15, 2012.
3. Basrak Z: Energy deposition in heavy-ion reactions at intermediate energies. International Workshop on Nuclear Symmetry Energy and Reaction Mechanisms (ASY-EOS 2012), Syracusa, Sicily, Italy, September 4-7, 2012.
4. Bogdanović Radović I: ASON-2, 2nd Adriatic School of Nanoscience, Dubrovnik, Croatia, September 2-7, 2012.
5. Brigljević, V: W and Z Physics with CMS, LHC Days in Split, Split, Croatia, October 1-6, 2012.
6. Fazinić S: High Resolution K X-ray PIXE spectra of 3d transition metals and their compounds, 22nd International Conference on the Applications of Accelerators in Research and Industry, Fort Worth, Texas, USA, August 5-10, 2012.
7. Gašparić I: The NeuLAND detector of the R3B collaboration. International Workshop on Nuclear Symmetry Energy and Reaction Mechanisms (ASY-EOS 2012), Syracusa, Sicily, Italy, September 4-7, 2012.
8. Jakšić M: Review of nuclear microprobe applications in materials science, 13th International Conference on Nuclear Microprobe Technology and Applications, Lisbon, Portugal, July 22-27, 2012.
9. Jakšić M: Ordering of nanostructures using MeV heavy ion microbeams, IUMRS-International Conference on Electronic Materials (IUMRS-ICEM 2012), Yokohama, Japan, September 22-29 2012.
10. Jakšić M: Joint ICTP-IAEA Workshop on Physics of Radiation Effect and its Simulation for Non-Metallic Condensed Matter, Trieste, Italy, August 13-24, 2012.
11. Krajcar Bronić I: Radiocarbon dating of St. Stephen's in Pustijerna church in Dubrovnik, Croatia. 3rd Symposium of the Balkan Archaeometry Network, Bucharest, Romania, October 29-30, 2012.
12. Soić N: Experimental research programme of Zagreb group on structure of light nuclei. International Workshop on Ab initio understanding of light nuclei, Birmingham, United Kingdom, December 12-13, 2012.
13. Stipčević M: Quantum random number generators and their applications in cryptography. SPIE Defense, Security, and Sensing, Baltimore, Maryland, USA, April 23-27, 2012.
14. Szilner S: Transfer reaction studies with spectrometers. 47th Zakopane Conference on Nuclear Physics, Zakopane, Poland, August 27- September 2, 2012.

SELECTED ORGANIZED CONFERENCES

1. The international conference *Nuclear Structure and Dynamics*, organized by the Physics Department of University of Zagreb and the Laboratory for Nuclear Physics of Ruđer Bošković Institute, co-chaired by D. Vretenar and S. Szilner, was held in Opatija, Croatia, on July 9-13, 2012. The conference gathered about 150 researchers and students from all around the world offering a review of recent experimental and theoretical advances in the physics of nuclear structure and reactions, and providing a broad discussion forum on current and future research projects. In the organization from RBI participated Zoran Basrak, Roman Čaplar, Tea Mijatović, Đuro Miljanić, Lovro Prepolec, Neven Soić, Suzana Szilner, Vedrana Tokić.

2. Diamond Detectors – Development and Applications, 2nd RBI Detector Workshop, Plitvice Lakes, 7-10 May 2012, Joint workshop of FP7 project Particle detectors and Croatian-Japanese Co-operative Program on Advanced Materials, chaired by Milko Jakšić and Mladen Kiš
3. Development and Utilization of MeV SIMS, Dubrovnik, 21-25 May 2012, Joint technical meeting IAEA, FP7 project SPIRIT, Croatian-Japanese Co-operative Program on Advanced Materials, chaired by Tonči Tadić
4. Silicon Detector Workshop, Split, 8-10 October 2012, organized through the FP7 project Particle Detectors, chaired by Vuko Brigljević

SELECTED PUBLICATIONS

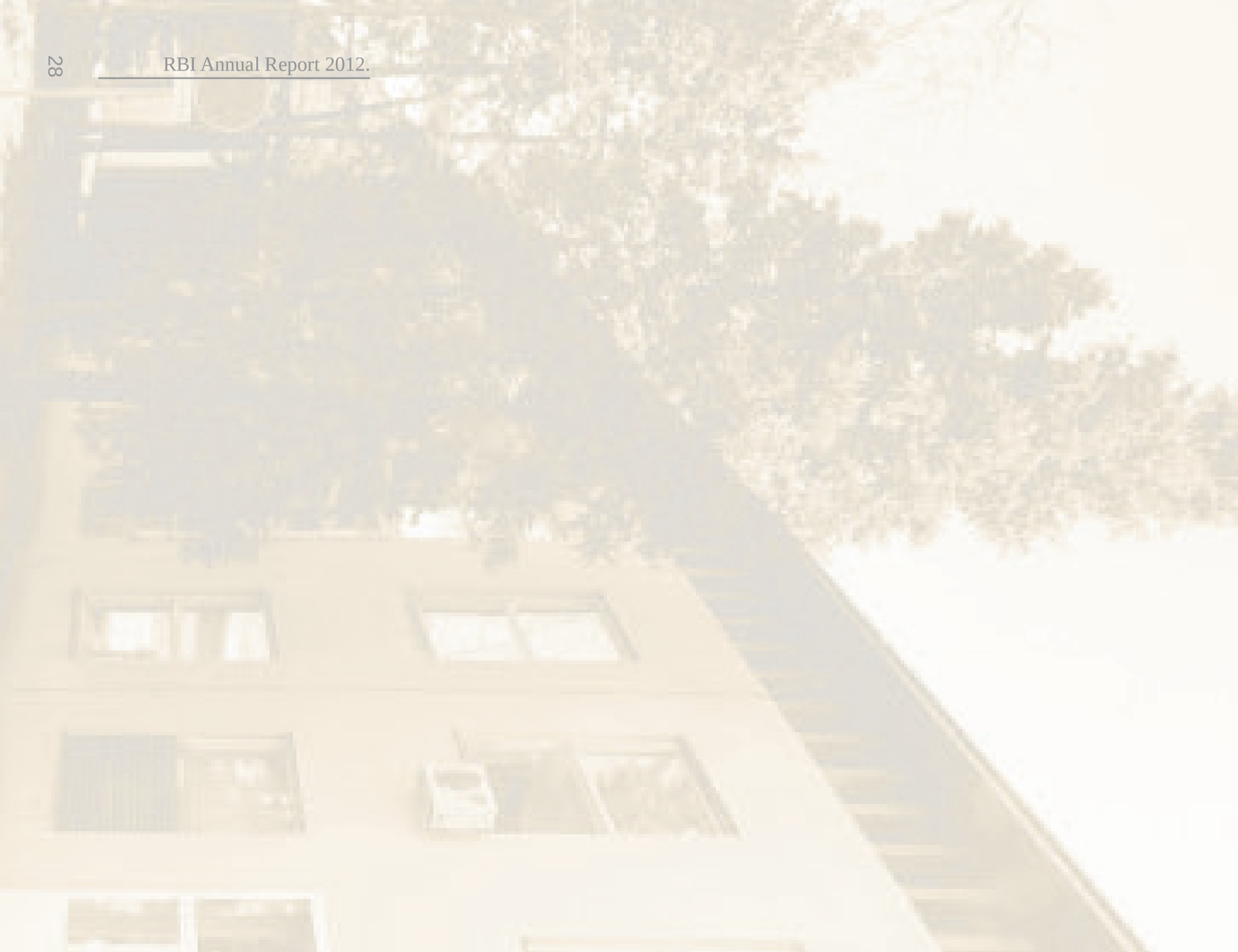
1. Horvat, R, Trampetić, J. A bound on the scale of spacetime noncommutativity from the reheating phase after inflation, *Phys Lett* **B710** (2012) 219-222.
2. Bogdanović-Radović I, Buljan M, Karlušić M, Skukan N, Božičević I, Jakšić M, Radić N, Dražič G, Bernstorff S. Conditions for formation of germanium quantum dots in amorphous matrices by MeV ions: Comparison with standard thermal annealing. Phys Rev **B86** (2012) 165316-1
3. Horvatinčić N, Krajcar Bronić I; Obelić B, Barešić J. Rudjer Bošković Institute radiocarbon measurements XVII. *Radiocarbon* **54** (2012) 137.
4. Valković V, Sudac D, Obhođaš J, Matika D, Kollar R, Nađ K, Orlić Z. Inspection of Objects on the Sea Floor Utilizing 14 MeV Tagged Neutrons. *IEEE Trans. Nucl. Sci.* **59/4** (2012) 1237-1244.
5. Abreu P. *et al.* (Pierre Auger Collaboration-RBI: Antičić T, Kadija K, Mičanović, S, Šuša T.). Measurement of the proton-air cross-section at s=√57 TeV with the Pierre Auger Observatory. *Phys Rev Lett* **109** (2012) 062002.
6. Abgrall N. *et al.* (NA61 Collaboration-RBI: Antičić T, Kadija K, Šuša T.) Measurement of production properties of positively charged kaons in proton-carbon interactions at 31 GeV/c. *Phys Rev* **C85** (2012) 035210.
7. Chatrchyan S. et. al. (CMS Collaboration-RBI: Brigljević V, **Đurić** S, Kadija K, Luetić J, Morović S.) A new boson with a mass of 125-GeV observed with the CMS experiment at the Large Hadron Collider, *Science* **338** (2012) 1569-1575.
8. Chatrchyan S. *et. al.* (CMS Collaboration-RBI: Brigljević V, Đurić S, Kadija K, Luetić J, Morović S.) Search for a W' or Techni-ρ Decaying into WZ in pp Collisions at sqrt(s)=7 TeV, *Phys Rev Lett* **109** (2012) 141801.
9. Adam T, et al. (OPERA collaboration-RBI: Jakovčić K, Kliček B, Ljubičić A, Stipčević M). Measurement of the neutrino velocity with the OPERA detector in the CNGS beam. *Journal of High Energy Physics* **10** (2012) 093-1.
10. Agafonova N, et al. (OPERA collaboration-RBI: Jakovčić K, Kliček B, Ljubičić A, Stipčević M). Momentum measurement by the multiple Coulomb scattering method in the OPERA lead-emulsion target. *New Journal of Physics* **14** (2012) 013026-1.
11. Agafonova N, et al. (OPERA collaboration-RBI: Jakovčić K, Kliček B, Ljubičić A, Stipčević M). Search for muon to tau neutrino oscillation with the OPERA experiment in the CNGS beam. *New Journal of Physics* **14** (2012) 033017-1.
12. Aleksić J, et al., (MAGIC Collaboration-RBI: Hrupec D, Surić T, Šnidarić I) Phase-resolved energy spectra of the Crab pulsar in the range of 50-400GeV measured with the MAGIC telescopes, Astronomy & Astrophysics 540 (2012) A69
13. Bottoni S et al. (RBI: Szilner S). Reaction dynamics and nuclear structure of moderately neutron-rich Ne isotopes by heavy-ion reactions. *Phys Rev* **C85** (2012) 064621.
14. Di Pietro A et al. (RBI: Zadro M). Experimental study of the collision ^{11}Be + ^{64}Zn around the Coulomb barrier. *Phys Rev* **C85** (2012) 054607.
15. Freer M et al. (RBI: Soić N). Resonances in ^{11}C observed in the ^{4}He(^{7}Be, α)^{7}Be and ^{4}He(^{7}Be, p)^{10}B reactions. *Phys Rev* **C85** (2012) 014304.
16. Montagnoli G et al. (RBI: Szilner S). Fusion of ^{40}Ca+^{40}Ca and other Ca+Ca systems near and below the barrier. *Phys Rev* **C85** (2012) 024607.
17. Montanari D el al. (RBI: Szilner S). γ spec-

troscopy of calcium nuclei around doubly magic ^{48}Ca using heavy-ion transfer reactions. *Phys Rev* **C85** (2012) 044301

18. Recchia F et al. (RBI:Szilner S). Spectroscopy of odd-mass cobalt isotopes toward the N=40 subshell closure and shell-model description of spherical and deformed states. *Phys Rev* **C85** (2012) 064305.
19. Zehr F et al. (Crystal Ball Collaboration-RBI: Korolija M, Mekterović D, Mićanović S, Supek I),Photoproduction of pi0 pi0 and pi0 pi± pairs off the proton from threshold to the second resonance region. *Eur Phys J* **A48** (2012) 98-116.
20. Kashevarov VL et al. (Crystal Ball Collaboration-RBI: Korolija M, Mekterović D, Mićanović S, Supek I), Study of the gamma p -> pi0 pi0 p reaction with the Crystal Ball/TAPS at the Mainz. *Phys Rev* **C85** (2012) 064610-064612
21. Pheron F et al. (Crystal Ball Collaboration-RBI: Korolija M, Mekterović D, Mićanović S, Supek I), Coherent photoproduction of η-mesons off ^{3}He – search for η-mesic nuclei. *Phys Lett* **B709** (2012) 21-27.

Book chapter

1. Special issue: Fizika B, 20 (2011) - Selected papers presented at the Third International Conference on Nuclear and Particle Physics with CEBAF at Jefferson Lab, urednici: I. Filikhin, I. Supek i B. Vlahović, Croatian Physical Society, Zagreb, 2012 (Proceedings).



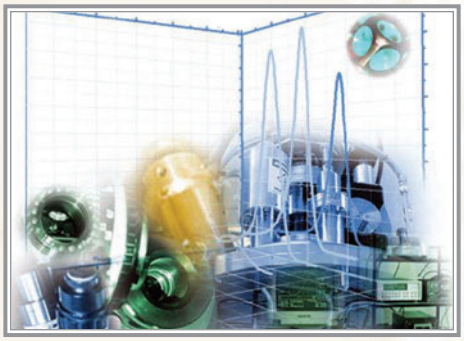
Division of Materials Physics

DIVISIONAL ORGANIZATION

Head: Branko Šantić

The Division of Materials Physics (ZFM) consists of the following laboratories:

- Laboratory for Semiconductors, Branko Pivac
- Laboratory for Thin Films, Nikola Radić
- Laboratory for Molecular Physics, Mile Ivanda



OVERVIEW OF THE DIVISION

The main areas of research in the division focus on the basic science of materials, particularly semiconductors, thin films and molecular physics. In addition, the division is involved in various applications oriented studies and activities. Several advanced experimental setups for the growth of samples and complex structures exist in the department. Various experimental techniques are used in the characterization of samples leading to explanations of their properties at the molecular and atomic scale. Some scientists are involved in theoretical modeling and numerical simulations, either in order to explain experimental results, or to suggest new directions of research and/or applications. Division members are active in numerous joint research projects, both at the national and international level.

TOP ACHIEVEMENTS

Doped optoelectronic and ceramic nanomaterials

The influence of doping atoms on the structure and microstructure of nanocrystalline optoelectronic materials was studied in order to explain and improve their physical properties. We have been focussed on doped luminescent materials that can be used as the active media for solid-state lasers, as well as cathodoluminescent materials. In order to improve and facilitate the investigation of microstructure, we are developing new software for analyzing the diffraction-line broadening.

Structure, microstructure and photoluminescence of nanocrystalline Ti-doped $ZnAl_2O_4$

Titanium doped $ZnAl_2O_4$ (gahnite) samples were successfully prepared for the first time. They were synthesized by a sol-gel technique. Samples were nanocrystalline with particles of ~20 nm in size. On doping titanium entered into the gahnite structure

as a Ti^{4+} ion, substituting for octahedral Al^{3+}. Doped samples exhibited luminescence under excitation in the UV absorption region (λ_{exc}=308 nm). Deconvolution of PL spectra indicated the existence of four luminescence bands with peaks at ~400, ~430, ~500 and ~520 nm, respectively. Intensities of emission bands were governed by Ti-doping level (Vrankić et al., 2012).

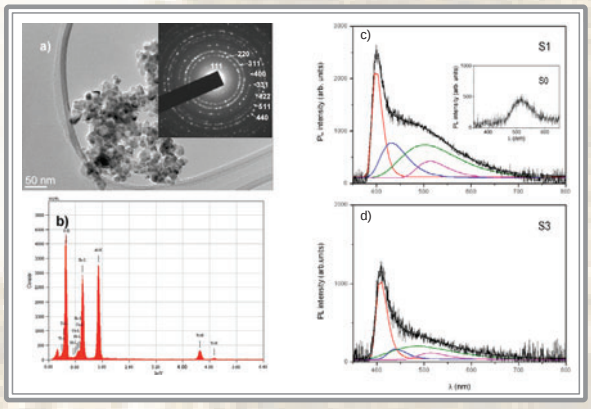


Fig. 1. (a) TEM bright-field image of gahnite sample S3 doped with 5.4 at% Ti in relation to Al, with the corresponding selected-area electron diffraction (SAED) pattern given in the inset; (b) EDXS spectrum of the sample S3; (c) PL spectrum of sample S1 (1.8 at% Ti) with spectrum of pure $ZnAl_2O_4$ (sample S0) in the inset; (d) PL spectrum of sample S3.

XBroad: program for quick determination of microstructural properties of materials

Nowadays, preparation of nanomaterials with controlled particle size and shape has been found to be essential for tailoring the desired material properties, so a quick and effective microstructural analysis is an imperative. The *XBroad* computer program was developed for easy and quick determination of basic microstructural information from powder X-ray diffraction data. The program was successfully tested on the ceria sample (CeO_2), (Skoko et al., 2012).

Carrier storage in Ge nanoparticles produced by pulsed laser deposition

We performed electrical characterization of Ge nanoparticles (NPs) produced by pulsed laser deposition (PLD) at room temperature (RT) in Ar gas inert atmosphere using a shadowed off-axis deposition geometry. Our results show that functional thin films of crystalline Ge NPs embedded between thin alumina films can be obtained on p-type Si(100) substrates following a low temperature and short rapid thermal annealing (RTA) treatment. Metal–oxide–semiconductor (MOS) structures with and without Ge NPs embedded in the alumina were prepared for the electrical measurements. The results indicate a strong memory effect at relatively low programming voltages (±4 V) due to the presence of Ge NPs (Martin-Sanchez et al., 2012).

Application of percolation theory and fractal analysis provides information on monolayer structure

The lattice structure and in plane molecular organization of a Langmuir monolayer of amphiphilic material is usually determined from grazing incidence X-ray diffraction (GIXD) or neutron reflectivity. Based on our previous research a different approach and a method for determination of monolayer structure based on application of percolation

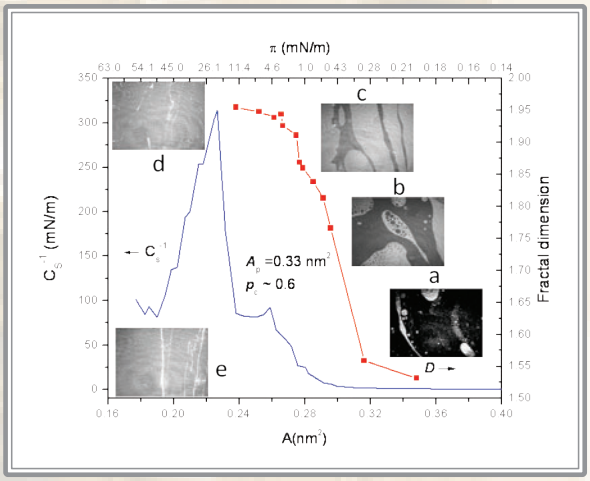


Fig. 2. Compressibility modulus and fractal dimension of a hexadecanol monolayer vs. area per molecule (A) and lateral pressure (π).The inserted BAM images show the monolayer structure at respective pressure/area range: (a) 0.2 mN/m; (b) 0.5 mN/m; (c) 1.3 mN/m; (d) 52.7 mN/m and (e) 61.3 mN/m.

theory and fractal analysis in combination with Brewster angle microscopy (BAM) has been developed and applied to the study of lipid monolayers (Risović et al., 2012).

Potential profile of quantum structures

It is usually assumed that the quantum step (QS), quantum well (QW) and quantum barrier (QB) have rectangular potential profiles. Our results show that the potential profiles are not rectangular. A quantum step is actually a smooth, gradual change of potential over a distance larger than one monolayer. For a narrow QW, instead of the quantum well, a more appropriate term is the quantum valley. The dipole layers formed by the ions and calculations of the electrostatic contribution to the potential were studied. Notably, the minimal thickness of the QS is not determined by the distance between the charged planes, but by the lateral spacing between ions of the same polarity. In the example of GaN, the QS cannot be thinner than about 3 Å (Šantić and Šantić, 2012).

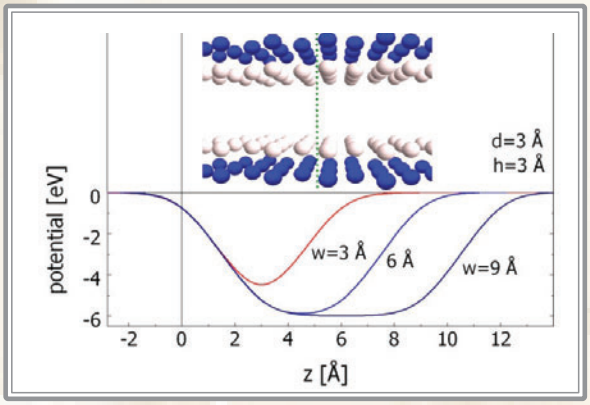


Fig. 3. Potential for the QW for the widths w=3 Å, 6 Å and 9 Å. INSET; QW composed of the two dipole layers. Potential is calculated along the z-axis (small green dots).

Quantum dots: GISAXS modelling and manipulation by ion-beam irradiation

We have developed theoretical models describing GISAXS grazing incidence small angle x-ray scattering) intensity distributions for three general classes of lattices of quantum dots (QDs). The method enables fast and accurate determination of material structure from the measured GISAXS maps [1]. Additionally, a method for the determination of ion track radii, formed in amorphous materials by ion-beam irradiation was developed in collaboration with the Laboratory for Ion Beam Interactions [2]. Comparison of the separations between the clusters that are formed by ions with different properties in the same type of material enables the determination of ion-track radii (Buljan et al., 2012).

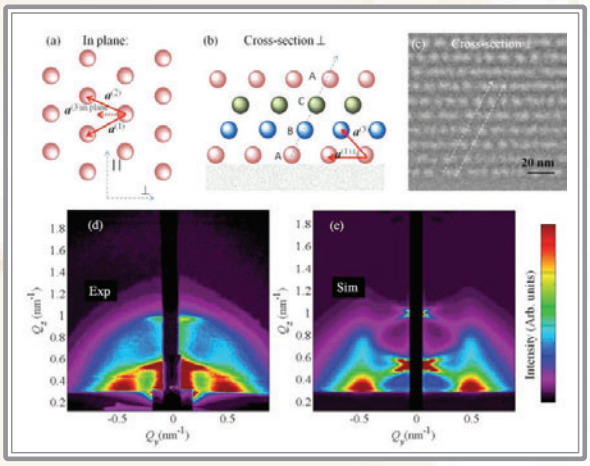


Fig. 4. (a),(b) Schematic views of the QD arrangement in the QD lattice formed during self-assembled growth of a (Ge+SiO_2)/SiO_2 multilayer. The lattice formed has a three-dimensional rhombohedral structure with the [111] axis perpendicular to the sample surface and it is described by basis vectors a_1-a_3 (indicated in the figure). (c) STEM image of the real (Ge+SiO_2)/SiO_2 multilayer film. (d), (e) Measured and simulated GISAXS maps from the same film, respectively.

Structural inhomogeneities in silicon-rich oxide thin films

Nonstoichiometric silicon oxide (SiO_x with x<2) thin films have been extensively studied during the last decades due to their importance in many electronic and optoelectronic applications. We studied the inhomogeneities in nonstoichiometric silicon oxide by a combination of different techniques. The oxygen content directly determined by TOF-ERDA,

EDX, ellipsometry and m-line measurements by using Bruggeman's EMA are much smaller than found by infrared absorption spectroscopy which is explained by inhomogeneities due to phase separation on the oxygen-rich SiO_y and silicon rich SiO_z (y>x>z) structures. This phase separation was further quantified by using X-Ray Photoelectron spectroscopy (XPS) technique. The XPS spectra of the Si 2p core levels clearly show an almost complete phase separation of the SiOx films into amorphous silicon and silica. These results, which indicate that in the analyzed samples the structure can be better described by the phase mixture model, can be of general utility to sustain the development of detailed analysis procedures aimed at improving the quality of silicon rich oxides films, where the oxygen content and its distribution play a crucial technological role. (Ristić, et al., 2012).

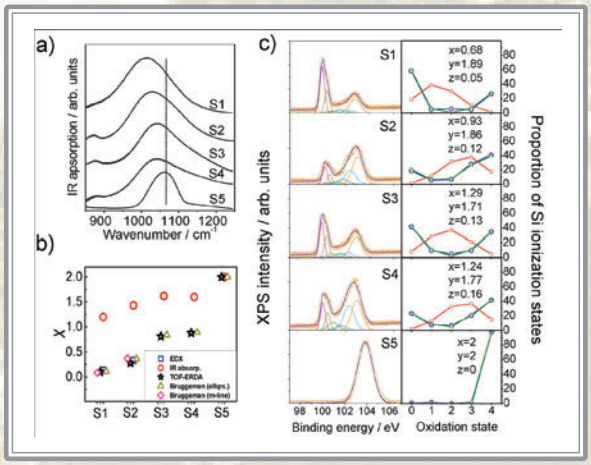


Fig. 5. (a) IR spectra of SiO_x thin films (samples S1-S5) deposited with LPCVD on silicon substrates. (b) The summarized results of the oxygen contents x obtained by TOF-ERDA, EDX, Bruggeman EMA and IR spectroscopy. The very good agreement between the first three techniques is evident. The oxygen content obtained from the IR spectra, however, appears much higher than all other values. This can be explained considering that the position of the Si-O stretching peak does not depend on the real oxygen content x, but on the microscopic amount of oxygen atoms around a given silicon atom. This means that estimation of the oxygen content by IR spectroscopy may suffer from non-negligible errors if the oxygen is non-homogeneously distributed in the sample network. In particular, if the oxygen atoms in a SiO_x matrix form SiO_y clusters (y > x), the oxygen content shown by the IR spectra would be equal to y rather than x. (c) The XPS spectra of the same samples S1-S5. In the left boxes the circles are the experimental XPS spectra, the dashed lines are the individual components of the Si 2p core level corresponding to different oxidation states of silicon, and the full line is their sum. In the right boxes the circles are the relative intensities of the individual components to the Si 2p core level, the squares are the calculated components according to the random-bonding model and the triangles are the calculated components according to the mixture model. The parameters used in the calculations are given inside the boxes.

EDUCATION

Members of the Division of Materials Physics were involved in teaching 10 undergraduate and 4 postgraduate courses of physics and related topics at the Faculty of Sciences, **Faculty of Electrical Engineering and Computing,** Faculty of Chemical Engineering and Technology in Zagreb and elsewhere.

AWARDS

Jasminka Popović received the Annual RBI Director's Award for excellence in scientific research and publishing in highly ranked scientific journals.

Igor Đerđ received the Annual RBI Director`s Award for excellence in scientific research and publishing in highly ranked scientific journals.

PROJECTS

Research program supported by the Ministry of Science, Education and Sports

1. Advanced materials and applications for energy conversion and storage, Branko Pivac

Research projects supported by the Ministry of Science, Education and Sports

1. Synergy of nanophases and nanocomposites, Maja Buljan
2. Basic properties of nanostructures and de-

fects in semiconductors and dielectrics, Branko Pivac
3. Doped optoelectronic and ceramic nanomaterials, Biserka Gržeta
4. The thin film silicon alloys on the amorphous to crystalline transition, Davor Gracin
5. Thin Films of Novel Amorphous or Nanostructured Materials, Nikola Radić
6. Semiconductor materials for optoelectronics and nanotechnology, Branko Šantić
7. Physics and application of nanostructures and bulk matter, Mile Ivanda
8. Organizational processes and optical interactions in condensed molecular systems, Dubravko Risović

Research, developmental and international projects

1. FP-7 NanoPV—Nanomaterials and nanotechnology for advanced photovoltaics, B. Pivac
2. UKF grant Nano - structural materials for thin film solar cells, D.Gracin/D. Balzar
3. COST Action MP 0901: Designing Materials for Nanodevices – from Theory to Practice, I. Capan
4. Structural characterization of novel complex materials with potential application, Igor Đerđ (Bilateral, Croatia-Montenegro)
5. Structural characterization of novel doped metal oxides nanoparticles, Igor Đerđ, (Bilateral, Croatia- Serbia)
6. Synthesis and characterization of novel metal oxides in ionic liquids, Igor Đerđ (DAAD, Croatia- Germany)
7. Doping semiconductor nanocrystals by neutron transmutation method, I. Capan (Bilateral, Croatia-Slovenia)
8. Comparison between electrical and structural properties of doped germanium nanocrystals, I. Capan (Bilateral, Croatia-Germany)
9. New nanostructural materials for thermoelectrics, Mile Ivanda (Bilateral, Croatia- Slovenia)
10. Structure and properties of functionalized one-dimensional titanate nanostructures designed for gas sensing application, Andreja Gajović (Bilateral, Croatia-Germany)

SELECTED ORGANIZED CONFERENCES

1. 14th Joint Vacuum Conference/ 12th European Vacuum Conference/ 11th Annual Meeting of the Deutsche Vakuum Gesellschaft/ 19th Croatian - Slovenian Vacuum Meeting (JVC-14/EVC-12/AMDVG-11/CroSloVM-19, www.jvc-evc-2012.com) Dubrovnik, Croatia, June 4-8, 2012 (Nikola Radić, Branko Pivac, Ivana Capan, Maja Buljan, Pavo Dubček).
2. ASON-2 - 2nd Adriatic School of Nanoscience, Dubrovnik, Croatia, September 2-7, 2012 (Mile Ivanda, Maja Buljan, Ivana Capan, Nikola Radić, Vedran Đerek).

SELECTED PUBLICATIONS

1. Vrankić M, Gržeta B, Mandić V, Tkalčec E, Milošević S, Čeh M, Rakvin B., Structure, mikrostructure and photoluminescence of nanocrystalline Ti-doped gahnite. *J Alloys Compd* **543** (2012) 213.
2. Skoko Ž, Popović J, Dekanić K, Kolbas V, Popović S. XBroad: program for extracting basic microstructure information from X-ray diffration patterns in few clics. *J Appl Cryst* **45** (2012) 594.
3. Kurajica S, Popović J, Tkalčec E, Gržeta B, Mandić V. The effect of annealing temperature on the structure and optical properties of sol-gel derived nanocrystalline cobalt aluminate spinel. *Mat Chem Phys* **135** (2012) 587.
4. Djerdj I, Popović J, Stare J, Ambrožić G, Škapin S D, Kozlevčar B, Pajić D, Jagličić Z, Crnjak Orel Z. Nanocrystalline hybrid inorganic-organic one-dimensional chain systems tailored with 2 and 3-phenyl rings monocarboxylic acids. *J Mat Chem* 22 (2012) 10255.
5. Djerdj I, Škapin SD, Čeh M, Jagličić Z, Pajić D, Kozlevčar B, Orel B, Crnjak Orel Z. Interplay between the Structural and Magnetic Probes in Elucidation of the Structure of Novel 2D Layered V4O4(OH)2(O2CC6H4CO2)4·DMF, *Dalton Trans* **41** (2012) 581.
6. Haetge J, Đerđ I, Brezesinski T. Nanocrystalline NiMoO4 with Ordered Mesoporous Mor-

phology as Potential Material for Rechargeable Thin Film Lithium Batteries. *Chem Commun* **48** (2012) 6726.
7. Reitz C, Suchomski C, Haetge J, Leichtweiss T, Jagličić Z, Djerdj I, Brezesinski T. Soft-Templating Synthesis of Mesoporous Magnetic CuFe2O4 Thin Films with Ordered 3D Honeycomb Structure and Partially Inverted Nanocrystalline Spinel Domains, *Chem Commun* **48** (2012) 4471.
8. Martin-Sanchez J, Chahboun A, Gomes MJM, Rolo AG, Pivac B,Capan I. Carrier storage in Ge nanoparticles produced by pulsed laser deposition. *Phys Status Solidi-RRL* **6** (2012) 223.
9. Buljan M, Radić N, Bernstorff S, Dražić G, Bogdanović-Radović I, Holý V. Grazing incidence small angle x-ray scattering: application in study of quantum dot lattices. *Acta Cryst A* **68** (2012) 124.
10. Buljan M, Karlušić M, Bogdanović-Radović I, Jakšić M, Salamon K, Bernstorff S, Radić N. Determination of ion track radii in amorphous matrices formation of nano-clusters by ion-beam irradiation. *Appl Phys Lett* **101** (2012) 103112.
11. Pinto SRC, Buljan M, Marques L, Martin-Sanchez J, Conde O, Chahboun A, Ramos AR, Barradas NP, Alves E, Bernstorff S, Grenzer J, Mucklich A, Ramos MMD, Gomes MJM. Influence of annealing conditions on the formation of regular lattices of voids and Ge quantum dots in an amorphous alumina matrix. *Nanotechnology* **23** (2012) 405605.
12. Bogdanović-Radović I,Buljan M, Karlušić M, Skukan N, Božičević I, Jakšić M, Radić N, Dražić G, Bernstorff S. Conditions for formation of germanium quantum dots in amorphous matrices by MeV ions: Comparison with standard thermal annealing. *Phys Rev* B **86** (2012) 165316.
13. Ristić D, Ivanda M, Speranza G, Siketić Z, Bogdanović-Radović I, Marciuš M, Ristić M, Gamulin O, Musić S, Furić K, Righini GC, Ferrari M. Local site distribution of oxygen in silicon-rich oxide thin films: A tool to investigate phase separation. *J Phys Chem C* **116** (2012) 10039.
14. Marciuš M, Ristić M, Ivanda M, Musić S. Formation and microstructure of nickel oxide films. J *Alloys Compounds* **541** (2012) 238.
15. Risovic D, Frka S, Kozarac Z. The structure of percolating lipid monolayers. *J Colloid Interface Sci* **373** (2012) 116.
16. Šantić B, Šantić N. Potential profile of the quantum step in semiconductors and the example of GaN. *Semicond Sci Technol* **27** (2012) 085014.

SELECTED INVITED LECTURES

1. Buljan M. Formation of three dimensional quantum dot lattices in amorphous systems E-MRS 2012 Fall Meeting, Symposium H: Organized Nanostructures and Nano-objects: Fabrication, characterization and applications, Warsaw, Poland, September 17-21, 2012.
2. Pivac B. Nanomaterials for photovoltaics. Advanced workshop on solar energy conversion. Bucharest, Romania, May 21-23, 2012.

BOOK CHAPTERS

1. Mikac L, Ivanda M, Štefanić G, Musić S, Furić K, Car D. Thermal Investigation of Copper-Doped-Zirconia Nanoparticles. NanoFormulation, Tiddy G, Tan R (eds.). London: Royal Society of London, RSC, 2012. pp. 188-193.

Division of Laser and Atomic Research and Development

LAIR

http://www.irb.hr/en/zlair

DIVISIONAL ORGANIZATION

Head: Hrvoje Zorc

The Division of Laser and Atomic R&D (Zavod za laserska i atomska istraživanja i razvoj) consists of the following laboratories:

- Laboratory of Thin Films and Optics, Vesna Janicki
- Multipurpose workshops, Eduard Švegel

OVERVIEW OF THE DIVISION

The mission of the Division is to expand and strengthen the knowledge in the field of imaging and non-imaging optics, photonics and the fundamentals of optical thin films. Besides this, activities are directed to the application of those basic disciplines in the field of national security.

The Division is currently developing several strategic projects. Those include modelling of thin films mixtures using effective medium theories, research on plasmonic properties of metallic nanoclusters, use of plasmonic materials in optical multilayer design, characterization and modelling of very thin metallic layers, sparse component analysis and tensor factorization approach to feature extraction from multispectral images and protein and/or gene expression levels with applications in disease (cancer) diagnosis and biomarker identification, nonlinear decomposition of multichannel medical images with application in contrast enhancement of multi-phase CT image and multispectral images in pathology, independent component analysis based approach to dictionary learning for efficient representations of the images of natural scenes with applications in filling-in missing values and denoising of images corrupted by salt and pepper noise and consensus-based regression with applications in prediction of anti-tumor activity of virtual chemical compounds.

The Division has been participating in one strategic project in the field of national security, together with the partner from industry and in coordination with Ministry of Defence.

TOP ACHIEVEMENTS

Metal island film based structures for sensing using spectrophotometry and ellipsometry

Metal island films (MIF) are good candidates for sensors due to environment refractive index sensitive localized surface plas-

mon resonance (SPR). The strong near field enhancement in the vicinity of the island surface can be even higher if metal layer (ML) is placed close to MIF. Structures containing MIF with (AuMIF*) and without ML (MIF*) were prepared and sensitivities of spectrophotometric and ellipsometric features of the measurements compared. It was shown that simple MIF is preferable for ellipsometric and the one including ML for spectrophotometric sensing.

Overall, AuMIF* structure is preferable for sensing in the case of spectrometric measurements, while ellipsometric measurements give advantage to MIF* structures having high values of spectral shift sensitivity. Those results offer a guideline for design of MIF based sensing structures depending on the availability of optical measurements.

Determination of percolation threshold and ageing of metal island films

Percolation threshold of Au island films, deposited on bare glass substrate or on pre-deposited Ge was studied. It was shown that the threshold for island percolation on Ge was shifted towards lower values of deposited material compared to the bare substrate. The result has been verified for unheated and preheated substrates. Finally, the change of optical properties with ageing was studied as well.

Blind data analysis

Research efforts were focused on methods for blind (a.k.a. unsupervised) data analysis with an emphasize on methods for: factorization of multidimensional arrays (tensors), factorization of nonlinear mixture models in reproducible kernel Hilbert spaces (RKHS), bases learning algorithms for filling in missing data and denoising. Tensor factorization methods have been applied to multidomain feature extraction for automated diagnosis of melanoma as well as for feature extraction from 1D datasets in proteomics and genomics. Nonlinear factorization methods have been applied to decomposition of multi-phase computed tomography (CT) images of an abdomen for segmentation of liver. Results obtained on clinical CT images were competitive, in terms of accuracy, with those obtained by state-of-the-art supervised graph-cuts algorithm. Nonnegative matrix factorization methods have been use to formulate new algorithm for fusion of remotely sensed multispectral and hyperspectal images.

PATENTS

1. US Patent 8,165,373. Kopriva I., Jerić I. Method of and system for blind extraction of more pure components than mixtures in 1D and 2D NMR spectroscopy and mass spectrometry combining sparse component analysis and single component points.
2. US Patent 8,224,427. Kopriva I. Method for real time tumour visualisation and demarcation by means of photodynamic diagnosis.

EDUCATION

Division members teach at the Faculty of Science, University of Zagreb,Faculty of Electrical Engineering and Computing, University of Zagreb, University of Applied Sciences Velika Gorica, and Karlovac University of Applied Sciences.

AWARDS

Award to Ivica Kopriva: The Annual award of the RBI Director for US patents 8,165,373 and 8,224,427 with the award for the granted project by Croatian Science Foundation entitled “Nonlinear component analysis with applications in chemometrics and pathology”.

PROJECTS

Projects supported by the Ministry of Science, Education and Sports

1. Analysis of multispectral data, Ivica Kopriva
2. Optical properties of nanostructured films, Hrvoje Zorc

SELECTED INVITED LECTURES

1. Kopriva I: Tensor Factorization: blind separation of multidimensional sources and feature extraction, University of South Toulon-Var, Toulon, France, April 19, 2012.

SELECTED PUBLICATIONS

1. Janicki V, Sancho-Parramon J, Yulin S, Flemming M, Chuvilin A. Optical and structural properties of Nb2o5-Sio2 mixtures. *Surf Coat Tech* **206** (2012) 3650.
2. Sancho-Parramon J, Bosch S. Dark modes and fano resonances in plasmonic clusters excited by cylindrical vector beams. *Acs Nano* **6** (2012) 8415.
3. Tikhonravov A, Amotchkina T, Trubetskov M, Francis R, Janicki V, Sancho-Parramon J, Zorc H, Pervak V. Optical characterization and reverse engineering based on multiangle spectroscopy. *Appl Optics* **51** (2012) 245.
4. Amotchkina T, Trubetskov M, Tikhonravov A, Janicki V, Sancho-Parramon J, Razskazovskaya O, Pervak V. Oscillations in spectral behaviour of total losses (1-R-T) in thin dielectric films. *Opt Express* **20** (2012) 16129.
5. Baršić G, Mahović S, Zorc H. Development of nano-roughness calibration standards. *Meas Sci Technol* **23** (2012) 035009.

Division of Electronics

DIVISIONAL ORGANIZATION

Head: Tomislav Šmuc

The Division of electronics consists of two laboratories and one research group:

- Laboratory for information systems, Dragan Gamberger
- Laboratory for stochastic signals and processes research, Branka Medved Rogina
- Computational biology and bioinformatics group, Tomislav Šmuc

OVERVIEW OF THE DIVISION

The mission of the Division of Electronics is to develop techniques and approaches capable of tackling data and information overload, a common problem for most scientific disciplines and contemporary technology environments. We develop techniques and approaches that blend signal processing, data handling, machine learning and data mining, with modern programming paradigms and knowledge technologies. Our main application disciplines include biomedical engineering, biology (genomics/proteomics), economics and social sciences. The Division has 15 staff members of which six are PhD students.

The members of the Division are involved in teaching courses at the Faculty of Electrical Engineering and Computing, the Faculty of Sciences and the School of Medicine at the University of Zagreb.

TOP ACHIEVEMENTS

Knowledge technologies and computer science

Large scale phyletic profiling-based protein-function prediction

To understand the deluge of genomic data we face, computational approaches for gene functional annotation are invaluable. We have recently introduced a novel model for computational protein function annotation based on the phyletic profiles of nearly a thousand prokaryotic genomes. The model is based on a novel multi-label classification algorithm and provides Gene Ontology function predictions for 998 prokaryotic genomes. The model includes more than 400,000 specific annotations with an estimated precision value of 90%; among these close to 19,000 are highly specific. This work will make experimental validation of predictions more efficient, both in terms of cost and time. A web resource based on the model is freely available to the research community at http://gorbi.irb.hr/ (Fig.1)

Fig. 1. GORBI WEB-service provides computationally predicted functional annotations for around a thousand sequenced prokaryotic genomes.

Object-oriented framework for data structures based on recursive automata

We have implemented a functionality for efficient finite state automata compression, as well as dictionary and lexicon components based on these data structures, into a software package that is easy to use, and extensible due to its object-oriented architecture. We continue to develop faster compression algorithms that will make the package a state of the art implementation of automata based dictionary compression. Parts of the package are useful as stand- alone components and the entire package can be used as a tool for both research and education. The finalized package will be published as open source software under a GPL license.

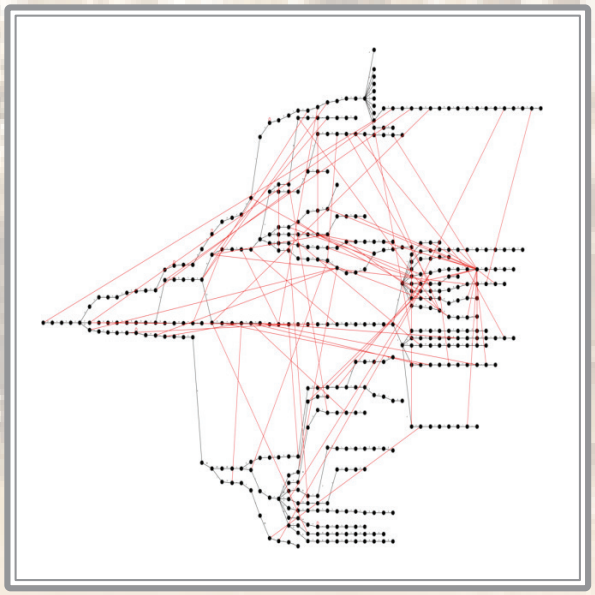


Fig. 2. Compressed tree automaton (lz-compression links are colored red)

Machine learning in complex systems/networks

Research in the field of complex systems/networks represents a new application area for the Division, and this startup phase coincides with our involvement in the FET project FOC (Forecasting Financial Crisis). We have developed a general statistical framework for the estimation of epidemic sources in arbitrary networks, which is currently a hot topic in the complex systems research community. Within the FOC project, we are working on the assessment of the impact of financial news and blogs on global systemic financial and economic risk. Besides developing new text processing based indicators, we will develop widgets that interactively visualize current risk in the near-real-time, relying on large-scale text processing developed by our partners on the project.

Using FPGAs to accelerate data mining tasks

We continue to explore implementation of some typical data mining algorithms in FPGA. Current implementations are mostly in the proof-of-concept stage and have not yet reached the maturity necessary for mainstream use. Our analysis has shown that FPGA is a very promising platform for running data mining tasks. The main focus of our current work is FPGA implementation of decision tree learning, the most commonly used technique in data mining. Accelerating

tree learning tasks will allow taking on larger datasets, as well as speeding up the model selection process. Current research efforts are focused on implementation in the Maxeler FPGA accelerator system.

Monography on rule learning

Dragan Gamberger has co-authored a book with Johannes Fuernkranz and Nada Lavrac, "Foundations of Rule Learning", one of the most comprehensive treatises in the field of rule learning. The book published by Springer, represents a unique source reference source for both researchers and students of computer science (Fig. 3).

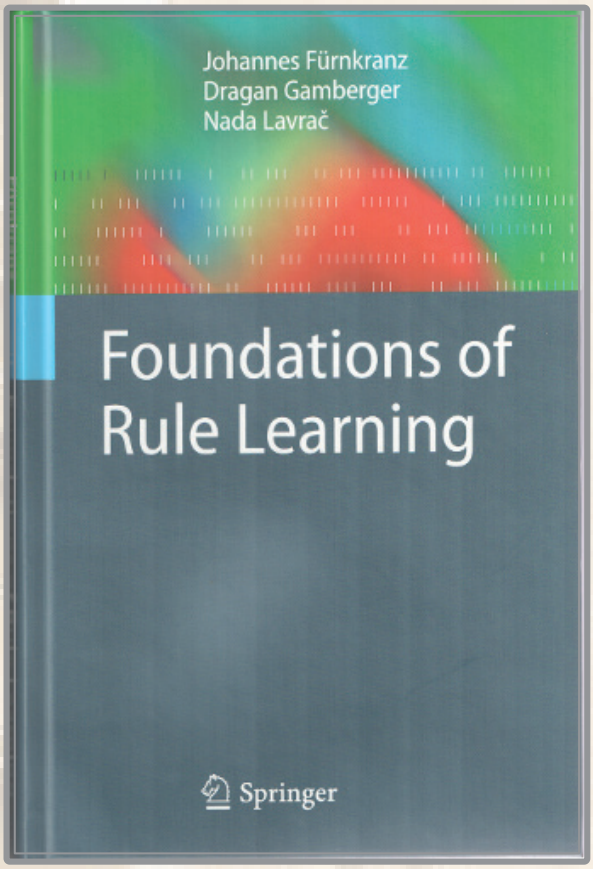


Fig. 3. New book "Foundations of Rule Learning" is one of the most thorough treatises in the rule learning field.

Signal processing techniques and measurement systems

Hand functionality assessment

Our long term research on the extraction of hand dynamics features, as well as new evaluation methods for hand functionality, has been enhanced with nonlinear time series measures. Embedding of symmetrically mirrored hand grip time series in a high dimensional phase space, results in a characteristic attractor of hand grip dynamics. Principal component analysis (PCA) is used to reveal the prevailing dimensionality of the underlying dynamics and to set the stage for invariant measure estimates. A modified procedure of approximate entropy (ApEn) calculation, with respect to PCA components, serves as the basis for hand functionality evaluation. The method has been tested and verified on healthy person's hand grip time series and on hand grips performed by patients with Rheumatoid arthritis (RA).

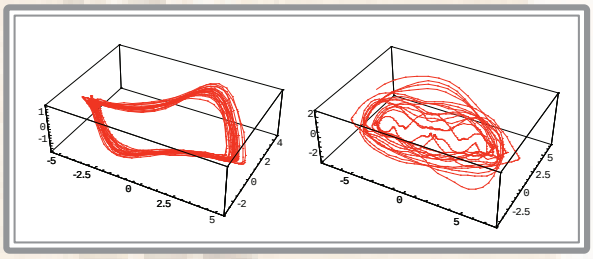


Fig. 4. Healthy hand grip (a) and Rheumatoid arthritis patient's (b) hand grip time series attractors.

EDUCATION

Educational activities in 2012 encompassed teaching undergraduate, graduate and doctoral courses at the Faculty of Electrical Engineering and Computing („Algorithms and Data Structures", S. Ristov), the Faculty of Sciences („Machine Learning", T. Šmuc) and School of Medicine of the University of Zagreb („Knowledge Discovery", D. Gamberger). Our division has also been involved in activities popularizing science. The Division's PhD students have been involved

in organization of the International Summer School of Science - S3 (http://s3.sci.hr/) for talented grammar school children, held in Višnjan, Croatia.

Projects supported by the Ministry of Science, Education and Sport

1. Machine Learning Algorithms and their Application, Dragan Gamberger
2. Computational Intelligence Methods in Measurement Systems, Ivan Marić
3. Real Life Data Measurement and Characterization, Branka Medved Rogina
4. Machine Learning of Predictive Models in Computational Biology, Tomislav Šmuc

Research, developmental and international projects

1. FOC - Forecasting Financial Crises (EU-FP7 FET Project), Tomislav Šmuc, Dragan Gamberger
2. Reconfigurable embedded systems based assistive applications for elderly people (Croatian-Hungarian Intergovernmental S&T Programme), Branka Medved Rogina

SELECTED PUBLICATIONS

Articles

1. Škunca N, Bošnjak M, Kriško A, Panov P, Džeroski S, Šmuc T, Supek F. Phyletic Profiling With Cliques of Orthologs is Enhanced by Signatures of Paralogy Relationships. *PLoS Comput Biol* **9** (2012) 1002852.
2. Ester K, Supek F, Majsec K, Marjanović M, Lembo D, Donalisio M, Šmuc T, Jarak I, Karminski-Zamola G, Kralj M. Putative mechanisms of antitumor activity of cyano-substituted heteroaryles in HeLa cells. *Invest New Drugs* **30** (2012) 450.
3. Krstačić G, Parati G, Gamberger D, Castiglioni P, Krstačić A, Steiner R. Heart rate variability and nonlinear dynamic analysis in patients with stress-induced cardiomyopathy. *Med Biol Eng Comp* **50** (2012) 1037.

Books

1. Fuernkranz J, Gamberger D, Lavrač N. Foundations of Rule Learning. Heidelberg: Springer, 2012.

Division of Physical Chemistry

http://www.irb.hr/en/str/zfk/

DIVISIONAL ORGANIZATION

Head: Aleksandar Sabljić

The Division of Physical Chemistry (ZFK) consists of the following laboratories:

- Laboratory for Chemical Kinetics and Atmospheric Chemistry, Branka Kovač
- Theoretical Chemistry Group, Slobodan Bosanac
- Laboratory of Chemical and Biological Crystallography, Marija Luić
- Laboratory for Magnetic Resonances, Boris Rakvin
- Laboratory for Synthesis and Processes of Selfassembling of Organic Molecules, Ivan Habuš

OVERVIEW OF THE DIVISION

The mission of the Division of Physical Chemistry is the discovery, exploitation, and dissemination of fundamental knowledge in the fields of protein science, coordination chemistry, spectroscopy, and computational and theoretical chemistry, in order to emerge as an internationally recognized Centre of Excellence in selected areas of molecular research.

In 2012. members of the Division have published nearly 50 contributions in atmospheric chemistry, chemical kinetics, structural chemistry, theoretical and computational chemistry, modelling of physical and chemical processes as well as in peptides and proteins research. A significant part is published in the highest ranking journals such as: The Journal of the American Chemical Society, Chemistry – A European Journal, Chemical Communications, Nucleic Acids Research, Physical Chemistry Chemical Physics, Dalton Transaction, Journal of Chemical Information and Modeling, Journal of Physical Chemistry A, Journal of Physical Chemistry C, Journal of Chemical Physics, Journal of Organic Chemistry, Journal of Medicinal Chemistry, FEBS Letters and CrystEngComm. A half of those contributions have been made within domestic and international collaborations. A number of fruitful international collaborations demonstrate strong presence of Division in the European Research Area. Division members also contribute extensively (about 30 courses) to undergraduate and graduate education in Croatia. Last but not least, division members organized the 13th BRIJUNI CONFERENCE – Space, Time and Matter a traditionally held international conference which included the participation of Nobel laureates. This highly regarded series of workshops has been supported by NATO and the Air Force Office of Scientific Research.

TOP ACHIEVEMENTS

Mechanisms of nonradiative deactivation in peptides

The mechanisms of nonradiative deactivation of a phenylalanine residue after near-UV photoexcitation have been investigated in an isolated peptide chain model (N-acetylphenylalaninylamide, NAPA) both experimentally and theoretically. Lifetime measurements at the origin of the first ππ* state of NAPA molecules have shown that among the three most stable conformers, the folded conformer NAPA B is nearly 50-times shorter lived than the extended major conformer NAPA A. Concurrent time-dependent density functional theory (TDDFT) based nonadiabatic dynamics simulations in the full dimensionality, carried out for the NAPA B conformer, provided direct insights on the novel classes of ultrafast deactivation mechanisms, proceeding through several conical intersections and leading in fine to the ground state. These results analyzed in the light of the experimental findings enabled us to assign the short lifetime of NAPA B conformer to a transfer of electronic excitation to a nπ* surface, induced by distortions of the backbone peptide bond (Mališ el al., 2012).

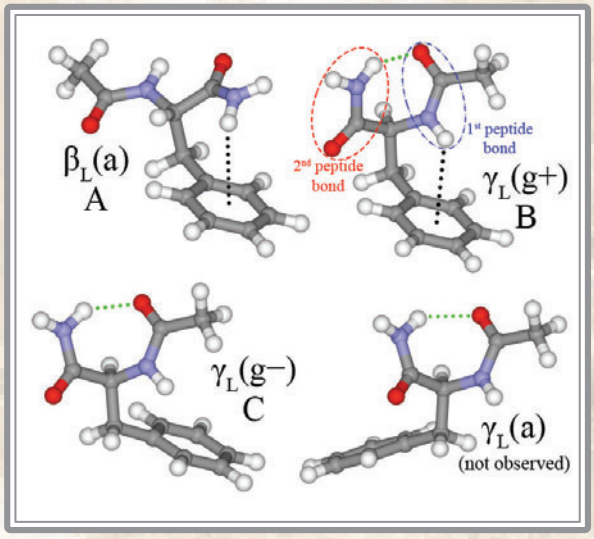


Fig. 1. Four most stable conformers of NAPA, together with their assignment to the experimentally observed conformers (A-C).

Biologically relevant metals

We have developed the Web-based platform for calculation of various statistical properties of metal-binding sites in biological macromolecules, proteins and nucleic acids (Tus et al., 2012). Currently, users can select up to 25 most representative metal ions to obtain the following statistical properties: presence of selected ligands in metal coordination sphere, distribution of coordination numbers, percentage of metal ions coordinated by the combination of selected ligands, distribution of monodentate and bidentate ASP/GLU ligands, percentage of particular binuclear metal centres, distribution of coordination geometries, descriptive statistics for a metal ion–donor distance and percentage of the selected metal ions coordinated by each of the selected ligands. Statistics are presented in numerical and graphical forms.

Fig. 2. Layout of the server homepage http://metals.zesoi.fer.hr

The large scale conformational change of the human DPP III

Extensive molecular modelling of human dipeptidyl peptidase III (DPPIII), a zinc−exopeptidase that hydrolyzes dipeptides from the N-terminus of its substrates, which consist of three or more amino acid residues has been performed. Using molecular dynamics we were able to trace large scale conformational changes of DPP III in solution, suggesting the pre-existing equilibrium model for a substrate binding. The amino acid residues most important for the enzyme conformational change, as well as those for binding of

ligands, were identified. The ligand binding modes were determined in the native protein and in its H568N mutant. The obtained results rationalized experimentally observed decreased catalytic performances of the mutant (Tomić et al., 2012).

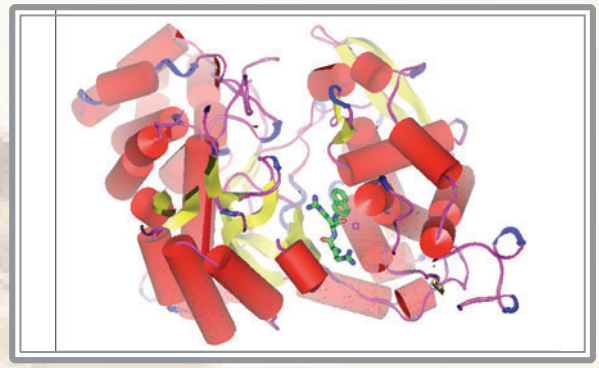


Fig 3. Substrate, Arg_2-2-naphtylamide, binding into the „closed" DPP III form. The complex was built using the enzyme structure obtained after 70 ns of MD simulations of the enzyme.

Effect of the BH_3 group on ligand–metal binding

Electronic structure of methylated azaferrocenes and their borane adducts, which are interesting as nucleophilic catalysts and ligands, conducting polymers and anticancer agents, have been investigated by UV photoelectron spectroscopy (UPS) and high-level DFT methods. Special attention was paid to geometry and electronic structure of dative bonds in donor-acceptor complexes which comprise an electron rich donor (Lewis base) and an electron deficient acceptor (Lewis acid). Electron localization function (ELF) calculations of the nitrogen basins were performed and the ELF isosurfaces (shown below) illustrate changes in the nitrogen lone pair upon donation to the borane. The results obtained by cyclic voltammograms and spectro-electrochemical characterization of some radical cations agree well with UPS data which allow us to suggest that UV-Vis transitions are of ligand-to-metal type (Brunker et al., 2012).

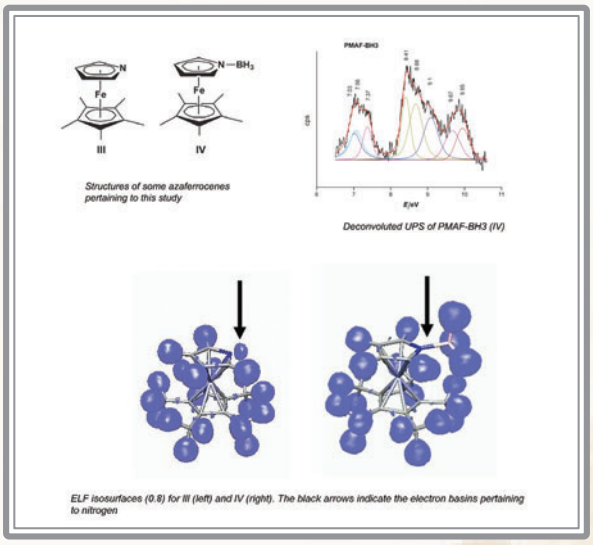


Fig 4. Molecular structures of azaferrocene (III) and azaferrocene-BH3 adduct (IV), deconvoluted UV photoelectron spectrum of IV and electron localization functions (ELF) for III and IV.

New approach in the synthesis of Ni(II) coordination compounds

In collaboration with the research group of M. Cindrić from the Faculty of Science solvent-based, electrochemical and mechanochemical methods have been applied in the synthesis of new Ni(II) thiosemicarbazone complexes interesting due to their po-

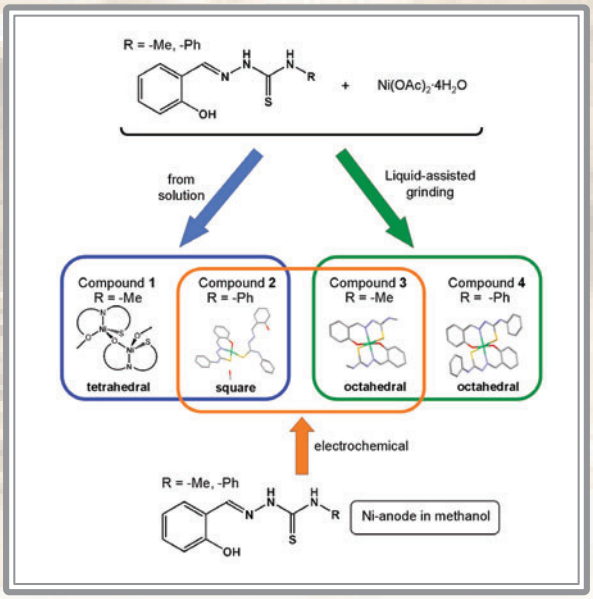


Fig 5. Different synthetic routes produce different thiosemicarbazonato complexes.

tential biological and catalytic activities. So far, in contrast to the solvent-based reactions, electrochemical and mechanochemical reactions have never been applied in the synthesis of Ni(II) thiosemicarbazonato complexes (Cindrić et al., 2012).

Temperature induced reversible structural and magnetic phase transitions in a crystal of tetrachlorosemiquinone anion radical

Magnetic properties of solvates of alkali salts of tetrachlorosemiquinone (chloranil) radical anion are tuned by crystal engineering using different solvents (2-butanone and acetonitrile) and/or cations (potassium and ammonium) in crystals. The structural and magnetic characteristics of two salts were studied by variable-temperature single crystal X-ray diffraction, magnetic susceptibility measurements, and calculations based on DFT or CAS-MP2 approach (Molčanov et al., 2012).

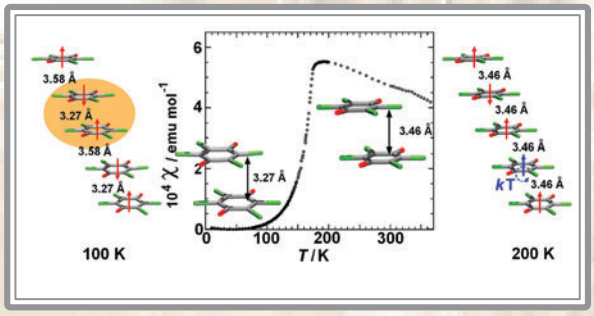


Fig 6. Temperature-induced, reversible monomer-dimer transition of potassium tetrachlorosemiquinone solvate in a crystal is accompanied by a change of magnetic properties of the two phases between the diamagnetic low-temperature phase and paramagnetic–like high-temperature phase.

Precipitation of calcium phosphates in the presence of titanate nanotubes

The influence of titanate nanotubes ($H_2Ti_3O_7$) on the formation and transformation of calcium phosphates has been investigated. Ability of nanotubes to induce formation of calcium phosphate in metastable solution was tested as well as the influence of nanotubes concentration on the rate of transformation, composition and morphology of the precipitates. The results have shown that titanate nanotubes are able to promote the formation of calcium phosphates from metastable solution and accelerate transformation of amorphous calcium phosphate to octacalcium phosphate. These investigations are important for the development of novel calcium phosphate based hybrid materials with improved mechanical properties (I. Bosak, B. Sc. Thesis, 2012).

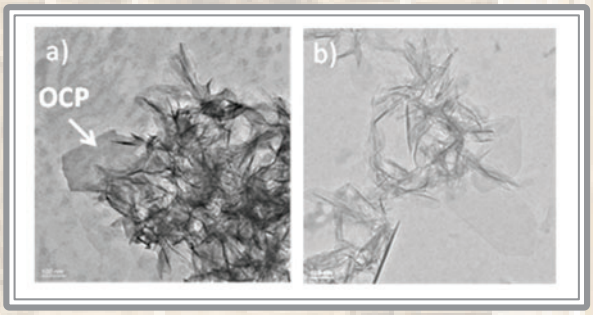


Fig 7. Calcium phosphates formed in the control system (a) and in the presence of titanate nanotubes after 24 hours (b).

EDUCATION

Division members provided more than 30 undergraduate and graduate courses at Universities in Zagreb, Split, Rijeka, Osijek and Dubrovnik.

AWARDS

1. Branka Kovač: Croatian Academy of Sciences and Arts (HAZU) award for scientific excellence.
2. Sanja Tomić: RBI Director's Prize for publishing in the highest ranking journals.
3. Maja Dutour Sikirić: RBI Director's Prize for publishing in the highest ranking journals.

PROJECTS

Program supported by the Ministry of Science, Education and Sport

1. Molecular structure, dynamics and reactivity. Program leader: Boris Rakvin

Projects supported by the Ministry of Science, Education and Sport

1. Molecular structure and dynamics of systems with paramagnetic particles, Boris Rakvin
2. Surfactants, processes in solutions and at interfaces, Maja Dutour Sikirić
3. Measurement and effect of atmospheric oxidants, Leo Klasinc
4. Advanced studies on chemical reactivity, Aleksandar Sabljić
5. Design, synthesis and properties of organic lignads and their metal complexes, Manda Ćurić
6. Protein-ligand interactions at atomic level, Marija Luić
7. Spectroscopy, chemical properties and reactions of biologically active molecules, Branka Kovač
8. Control of atomic and molecular dynamics by shaped electromagnetic fields, Nađa Došlić
9. Computational study of bio-macromolecules and development of new algorithms, Sanja Tomić
10. Development of mathematical methods for the description of molecular structure, dinamics and reactivity, Darko Babić
11. Amino-beta-lactams-synthrons for biologically interesting compounds, Ivan Habuš

Research, developmental and international projects

1. Multifunctional composite coatings for bone implants, M. Dutour Sikirić (BICRO, Proof of concept project)
2. Excited states of peptides in gas phase, I. Ljubić (Bilateral project with France, Program "COGITO")
3. Laser controlled switching of molecular photonic wires, N. Došlić (Bilateral project with Germany)
4. The study of condensed matter by EPR: Dynamics in glassy and crystalline matrices, M. Ilakovac Kveder (AvH research group linkage project)
5. Study of plant enzymes from metallopeptidase families M20 and M49, S. Tomić, M. Abramić, B. Salopek Sondi, B.J. Ludwig-Műller, R. Wade (AvH research group linkage project)
6. Supramolecular chemistry in water, M. Ilakovac Kveder (COST CM1005)
7. Advance ESR tehniques on chemistry, B. Rakvin (Bilateral project with Austria)
8. Synthesis, identificatrion and biological activity testing of novel beta lactam cholesterol absorption inhibitors, I. Habuš (Bilateral project with Austria)
9. Sythesis, structure, and antifungla activity of novel dithiocarbamato EDTA derivatives and their metal complexes, A. Višnjevac (Bilateral project with Montenegro)
10. Correlation of structural characteristics and physical properties of quinoid rings leads to novel functional materials, K. Molčanov (Bilateral project with Slovenia)
11. Computer program for mass spectrometry data reduction collected during protein cross-linking experiments, Saša Kazazić (HAZU project)

SELECTED INVITED LECTURES

1. Rakvin B (2012) The EPR Study of Trehalose Frozen-in Disorder. APES 2012, 8th Asia-Pacific EPR/ESR Symposium, Bejing, China, October 11-15, 2012.
2. Rakvin B (2012) Study of stable L-alanine radicals involved in alanine/ESR dosimetry by advanced ESR spectroscopes. Department of Radiological Life Sciences, Hirosaki University, Hirosaki, Japan, October 17, 2012.
3. Tomić S (2012) Molecular modeling of nucleic acid - small molecule interactions. Regional Biophysical Conference, Kladovo, Serbia, September 3-7, 2012.

4. Molčanov K (2012) Snails, mirrors and coordinate systems: a different way of teaching stereochemistry. 2nd Croatian Workshop on Chemical Education, Split, Croatia, November 8-11, 2012.

SELECTED PUBLICATIONS

1. Mališ M, Loquais Y, Gloaguen E, Biswal SH, Piuzzi F, Tardivel B, Brenner V, Broquier M, Jouvet C, Mons M, Došlić N, Ljubić I. Unraveling the mechanisms of nonradiative deactivation in model peptides following photoexcitation of a phenylalanine residue. *J Am Chem Soc* **134** (2012) 20340.
2. Rubčić M, Užarević K, Halasz I, Bregović N, Mališ M, Đilović I, Kokan Z, Stein RS, Dinnebier RE, Tomišić V. Desmotropy, polymorphism, and solid-state proton transfer: four solid forms of an aromatic o-hydroxy Schiff base. *Chem Eur J* **18** (2012) 5620.
3. Basarić N, Došlić N, Ivković J, Wang YH, Mališ M, Wan P. Very efficient generation of qinone methides through excited state intramolecular proton transfer to a carbon atom. *Chem Eur J* **18** (2012) 10617.
4. Matanović I, Kent PRC, Garzon FH, Henson NJ. Density functional theory study of oxygen reduction activity on ultrathin platinum nanotubes. *J Phys Chem C* **116** (2012) 16499.
5. Tomić A, Gonzalez M, Tomić S. The large scale conformational change of the human DPP III – substrate prefers the “closed” form. *J Chem Inf Model* **52** (2012) 1583.
6. Tus A, Rakipović A, Peretin G, Tomić S, Šikić M. BioMe: biologically relevant metals. *Nucleic Acids Res* **40** (2012) W352.
7. Aleksić M, Bertoša B, Nhili R, Uzelac L, Jarak I, Depauw S, David-Cordonnier MH, Kralj M, Tomić S, Karminski-Zamola G. Novel substituted benzothiophene-, thienothiophene-carboxanilides, quinolones: synthesis, photochemical synthesis, DNA–binding properties, antitumor evaluation, QSAR analysis. *J Med Chem* **55** (2012) 5044.
8. Brunker TJ, Kovač B, Kowalski K, Polit W, Winter RF, Rheingold AL, Novak I. Electronic structures of methylated azaferrocenes and their borane adducts: photoelectron spectroscopy and electronic structure calculations. *Dalton Trans* **41** (2012) 3675.
9. Ljubić I, Clary DC. Quasiclassical trajectory calculations of hydrogen absorption in the $(NaAlH_4)_2Ti$ system on a model analytical potential energy surface. *Phys Chem Chem Phys* **14** (2012) 3915.
10. Cindrić M, Uzelac M, Cinčić D, Halasz I, Pavlović G, Hrenar T, Ćurić M, Kovačević D. Three routes to nickel(II) salicylaldehyde 4-phenyl and 4-methylthiosemicarbazonato complexes: mechanochemical, electrochemical and conventional approach. *CrystEngComm* **14** (2012) 3019.
11. Molčanov K, Kojić-Prodić B, Babić D, Pajic D, Novosel N, Zadro K. Temperature induced magnetic bistability in a crystal of tetrachlorosemiquinone anion radical. *CrystEngComm* **14** (2012) 7958.

Division of Organic Chemistry and Biochemistry

http://www.irb.hr/en/zokb

DIVISIONAL ORGANIZATION

Head: Kata Majerski

The Division of Organic Chemistry and Biochemistry (DOCB) consists of the following laboratories:

- Laboratory for stereoselective catalysis and biocatalysis, Zdenko Hameršak
- Laboratory for synthetic organic chemistry, Kata Majerski
- Laboratory for supramolecular and nucleoside chemistry, Mladen Žinić
- Laboratory for carbohydrate, peptide and glycopeptide chemistry, Lidija Varga-Defterdarović
- Laboratory for cellular biochemistry, Marija Abramić
- Laboratory for physical organic chemistry, Davor Margetić
- Laboratory for molecular spectroscopy, Goran Baranović
- Laboratory for study of interactions of biomacromolecules, Ivo Piantanida
- Group for quantum organic chemistry, David Smith

OVERVIEW OF THE DIVISION

In 2012, the members of the Division continued to maintain their established excellence in scientific research. Our principal focus was basic research in the fields of organic and bioorganic chemistry. The Division published over 70 research articles, primarily in high-ranking chemical journals. Amongst the broad range of research topics, important contributions were made in areas such as synthetic and physical organic chemistry, mechanochemistry, stereoselective synthesis, supramolecular chemistry, including gels and host-guest interactions, the interactions of small molecules with DNA/RNA, the chemistry of peptides and peptidomimetics as well as experimental and computational protein biochemistry. In addition to fundamental research, 1 patent application was approved. Members of the Division provided significant contributions to higher education by participating in numerous courses at the undergraduate and graduate levels, as well as by supervising 9 Diploma and 2 PhD theses. The Division's staff were also active in national and international societies and bodies and served as editors or members of several editorial boards.

TOP ACHIEVEMENTS

Invited review article reporting recent progress in the fields of computational and experimental evaluation of basicity parameters and the design of novel superbases

This article, published in the highest impact-factor journal in chemistry, namely Chemical Reviews, provides an overview of research related to the interpretation of fundamental proton-transfer reactions and the design of new highly basic materials. It also summarizes more than 40 articles that members of the Quantum Organic Chemistry Group have published in the last decade in this lively and propulsive field of research (Maksić et al., 2012).

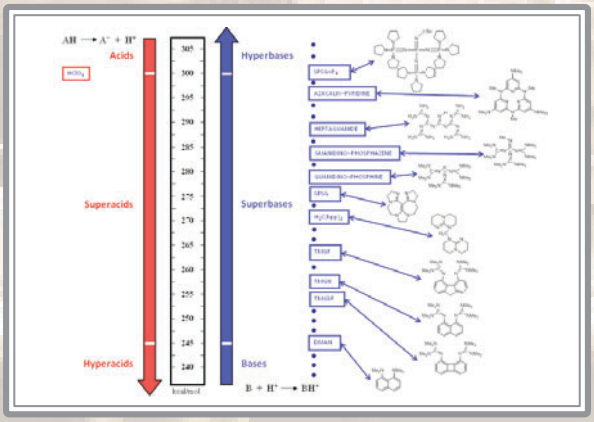


Fig. 1. Ladder of superbases and hyperbases in the gas-phase enabling unified and continuous scale of all acids and bases.

Crystal structure reveals an exceptional flexibility of human dipeptidyl peptidase III

The first crystal structure of human dipeptidyl peptidase III (DPP III), a physiologically important protease, and its complex with the opioid pentapeptide tynorphin has been determined. The two rigid lobes of the enzyme undergo an exceptionally large domain motion (a 60° rotation about a "hinge" region) upon ligand binding to form a closed active site. The interactions between the peptide and the DPP III protein are detailed, defining the amino acid residues constituting the peptide binding subsites. Microcalorimetric analyses have shown that peptide binding was strongly endothermic. This work, which is the result of interdisciplinary collaboration with scientists from the Institute of Molecular Biosciences and the Institute of Biochemistry from Graz, and the Structural Genomic Consortium, University of Toronto, establishes DPP III as one of a very few peptidases to display an entropy-driven binding mode and a large domain movement upon substrate binding (Bezerra et al., 2012).

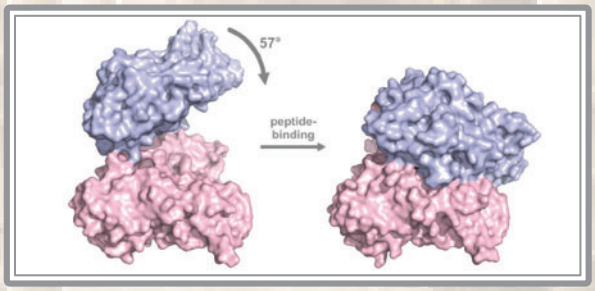


Fig. 2. Domain movement upon tynorphin binding to human DPP III. Surface representation of ligand-free enzyme (left) and of the peptide complex (right).

Spectrophotometric differentiation between various ds-DNA/RNA by interaction with small molecules

Studies of various aspects of DNA/RNA recognition by small organic molecules resulted in 10 scientific publications in Wos referenced journals, among which the most intriguing was efficient kinetic and chirooptical (induced CD) differentiation between dGdC, dAdT and rArU sequences by a novel cyanine dye (Tumir et al, 2012).

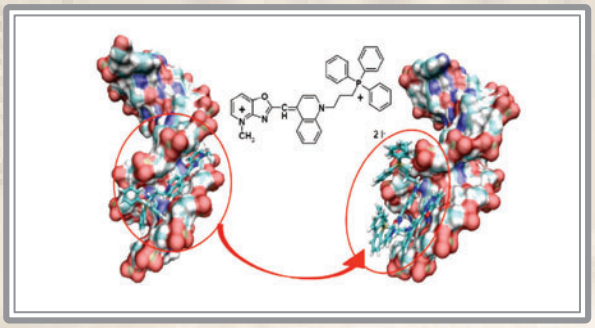


Fig. 3. The DNA-minor groove bound cyanine dye by transition from monomer (LEFT) to dimer (RIGHT) unwinds exclusively poly dA – poly dT sequence by uniquely slow kinetics.

Insight into features of the monoamine oxidase enzyme

Computational simulations performed on monoamine oxidase flavoenzyme revealed that (a) its active site is highly hydrophilic, but turns hydrophobic upon substrate binding, and (b) dopamine binds as a monocation with its pKa value allowing it to enter the chemical transformation in both neutral and protonated forms. These insights contradict traditional opinions on these features and provide crucial information for advancing current treatments against neurological diseases (Borštnar et al., 2012).

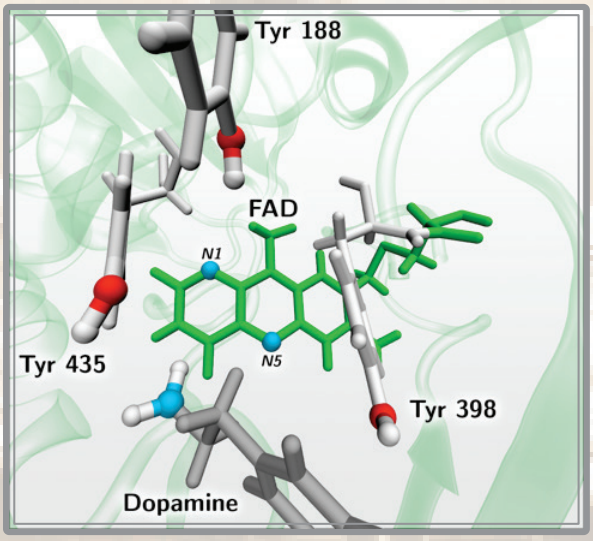


Fig. 4. Structure of the active site of monoamine oxidase enzyme in complex with dopamine.

Intermolecular central to axial chirality transfer in the self-assembled biphenyl containing amino acid–oxalamide gelators

Chiral amino acid and biphenyl incorporating oxalamide gelators 4–7 with large, 9 bond distance between chiral centers and biphenyl units have been studied. CD and NMR investigation of a 4-octanol gel and the crystal structure of *rac*-4 reveal that efficient central to axial chirality transfer occurs by intermolecular interactions in gel and solid state assemblies (Makarević at al., 2012).

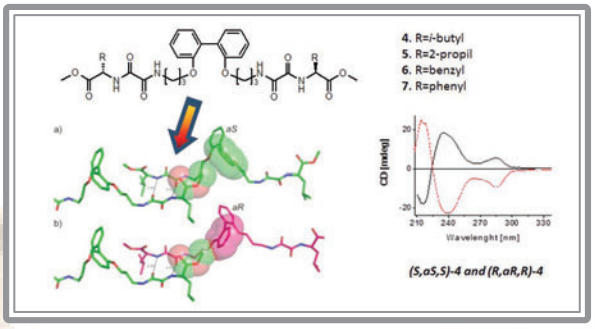


Fig. 5. (a) Biphenyl incorporating oxalamide gelators 4–7; (b) Molecular models of self-assembled (S,aS,S)- and (S,aR,S)-4 diastereoisomers showing the origin of specific central (S)- to axial (aS)- chirality transfer due to strong steric repulsion in the (S,aR,S)-4 diastereoisomers assemblies; (c) CD spectra of enantiomeric (S,aS,S)- and (R,aR,R)-4 showing central (S)- and (R)- to axial (aS)- and (aR)- chirality transfer, respectively.

A model for a solvent-free synthetic organic research laboratory: click-mechanosynthesis and structural characterization of thioureas without bulk solvents

The mechanochemical click coupling of isothiocyanates and amines has been used as a model reaction to demonstrate that the concept of a solvent-free research laboratory, which eliminates the use of bulk solvents for either chemical synthesis or structural characterization, is applicable to the synthesis of small organic molecules. The enhanced efficiency of electrical ball milling techniques, neat grinding or liquid-assisted grinding, over manual mortar-and-pestle synthesis is demonstrated in the synthesis of 49 different thiourea derivatives. Comparison of powder X-ray diffraction data of mechanochemical products with structural information found in the Cambridge Structural Database, or obtained herein through single crystal X-ray diffraction, indicates that the mechanochemically obtained thiourea derivatives are pure in a chemical sense, but can also demonstrate purity in a supramolecular sense, i.e. in all structurally explored cases the product consisted of a single polymorph. These results serve as the illustration for the cover page of Green Chemistry. (Štrukil et al., 2012).

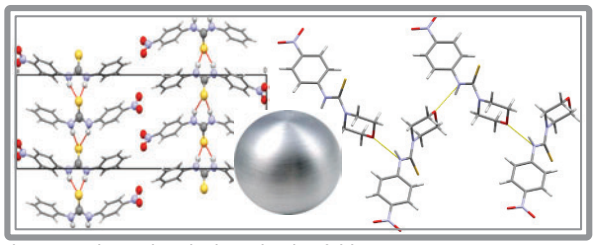


Fig. 6. Mechanochemical synthesis of thioureas.

Click mechanochemistry: quantitative synthesis of "ready to use" chiral organocatalysts by efficient two-fold thiourea coupling to vicinal diamines

Mechanochemical methods of neat grinding and liquid-assisted grinding have been applied to the synthesis of mono- and bis-thioureas using the click coupling of aromatic and aliphatic diamines with aromatic isothiocyanates. Quantitative reaction yields, combined with the fact that mechanochemical reaction conditions avoid the use of bulk solvents, enabled solution-based purification methods (such as chromatography or recrystallization) to be completely avoided. In this way, mechanochemical synthesis provides a facile way to fully transform valuable enantiomerically pure reagents into useful products that could be immediately applied for a designed purpose. This was demonstrated by using some of the mechanochemically prepared reagents as organocatalysts in a model Morita-Baylis-Hillman reaction and as cyanide ion sensors in organic solvents. These research results were selected as "Hot-topics" in the click-chemistry area (Štrukil et al., 2012).

Very excited state intramolecular proton transfer (ESIPT) to carbon atom

Irradiation of 2-phenyl-1-naphthol in CH_3CN-D_2O (3:1) leads to very efficient incorporation of deuterium at the *ortho* positions of the adjacent phenyl ring (overall Φ = 0.73±0.07), along with minor incorporation at naphthalene positions 5 and 8. Theoretical and experimental investigations give a rationale for the findings that involves the most efficient ESIPT from the phenol OH to the corresponding carbon atoms ever reported, thus giving rise to quinone methides (Basarić et al., 2012).

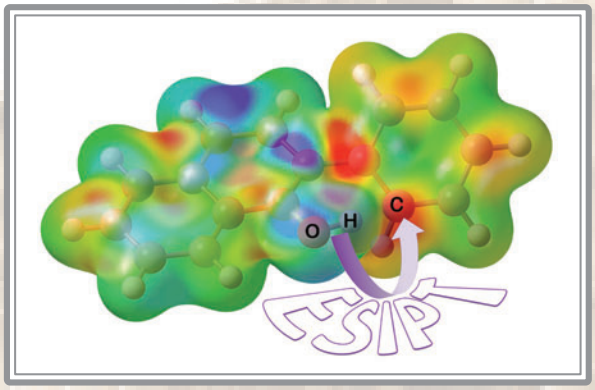


Fig. 7. Calculated difference in the electronic densities between ^1L_b and S_0 at the ^{1}Lb minimum energy geometry projected on the electron density surface of S_0 with isovalue of 0.01/ Å^3.

Characterization of sterically congested adamantylnaphthalene quinone methides and investigation of their antiproliferative activity

Five new (2-adamantyl)naphthol derivatives (quinone methide precursors) were synthesized and their photochemical reactivity investigated by preparative photolyses, fluorescence spectroscopy and laser flash photolysis. Antiproliferative activity was investigated on three human cancer cell lines with and without exposure to 300 nm irradiation (Veljković et al., 2012).

Catalytic activity of halohydrin dehalogenases towards spiroepoxides

A novel activity of halohydrin dehalogenases towards spiroepoxides has been found. The enzyme from Arthrobacter sp. catalysed highly regioselective azidolysis of spiroepoxides containing 5, 6 and 7-membered cycloalkane rings, while the enzyme from Agrobacterium radiobacter, in addi-

tion to a high regioselectivity, also displayed moderate to high enantioselectivity (E up to >200) that can be applied to the kinetic resolution of chiral spiroepoxides (Majerić Elenkov et al., 2012).

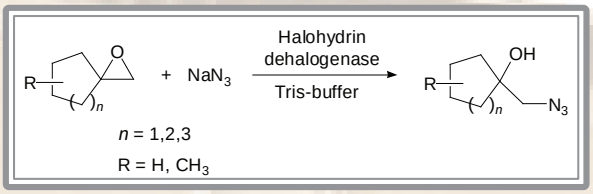


Fig. 8. Enzyme catalysed azidolysis of spiroepoxides.

Amino acid-based tweezers as copper(II) binding sites

We report the synthesis of conformationally constrained amino acid-based diamines and study of their affinity towards Cu(II). It was shown that these small molecular tweezers effectively mimic Cu(II) binding peptides, thus confirming the hypothesis that a turn-like conformation significantly contributes to Cu(II) binding efficiency (Gredičak et al., 2012).

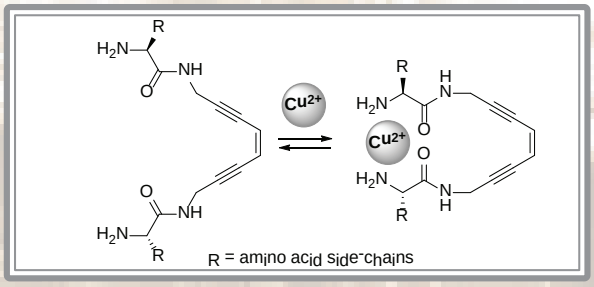


Fig. 9. Amino acid-based tweezers.

In vivo toxicity study of N-1-sulfonylcytosine derivatives and their mechanisms of action in cervical carcinoma cell line

An *in vivo* toxicity study of *N*-1-sulfonylcytosine derivatives was performed together with studies of their mechanisms of action in a cervical carcinoma cell line. Potent antitumor efficacy and low toxicity of new compounds in comparison with the common chemotherapy drug 5-FU make them promising anticancer agents (Kašnar-Šamprec et al., 2012).

Details of the catalytic mechanism of monoamine oxidase flavoenzyme

After several decades of persistent yet inconclusive research on monoamine oxidases (MAOs), the results of this work elucidated the precise molecular mechanism of how biogenic amines are metabolized by MAOs, enzymes responsible for regulating neurotransmitter levels in various parts of brain. These results are relevant for targeting neurological illnesses through the design of novel antidepressants and antiparkinsonian drugs as transition state analogues, and were illustrated on the cover page of *Eur J Org Chem* (Vianello et al., 2012).

Fig. 10. Cover page of the European Journal of Organic Chemistry depicting the rate-limiting first step in the monoamine oxidase-catalyzed degradation of biogenic amines in various parts of brain.

Ring-opening reactions in **adamantyl-β-butyrolactones**

The adamantane moiety plays an important function in lowering lactone reactivity by protecting electrophilic sites on the four-membered ring via steric hindrance. These novel lactones showed pronounced stability and were resistant to cleavage upon acidic water extraction and column chromatographic purification. However under certain conditions, both

O–C(carbonyl) and O–C(alkyl) bond-cleavage ring-opening reactions were observed. Bond-cleavage at physiological temperature makes these novel lactones especially noteworthy (Matković et al., 2012).

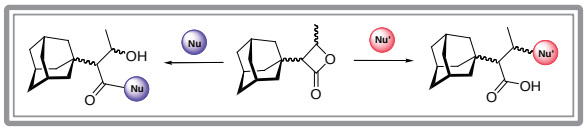


Fig. 11. Ring-opening reactions in different conditions.

DBU induced formation of 8-bromoguanosine dimer with three hydrogen bonds between the GG- pairs

Upon hemideprotonation of 8-bromoguanosine (8-BrG) at the N1 position induced by DBU, the adduct $[8\text{-BrG}][8\text{-BrG}]^{-}[\text{DBU-H}]^{+}$ was formed; its crystal structure and NMR results show that a 8-BrG dimer containing three hydrogen bonds is formed in the solid state and in DMSO solution despite high H-bond competitiveness of the solvent (Saftić et al., 2012).

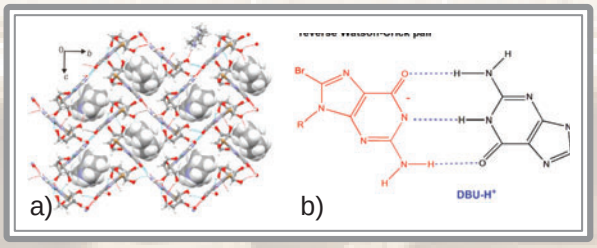


Fig. 12. Adduct [8-BrG][8-BrG]-[DBU-H]+: a) crystal structure showing the packing along a axis; b) DBU induced 8-BrG dimerization by three hydrogen bonds.

PATENT

US patent 8, 165, 373 B2. Kopriva I, Jerić I. Method of and system for blind extraction of more pure components than mixtures in 1D and 2D NMR spectroscopy and mass spectrometry combining sparse component analysis and single component points.

SPIN OFF COMPANY

BioZyne Ltd. was re-launched in 2010/2011 with a new research and development strategy in life sciences and chemistry. The company builds its own portfolio of optimized lead compounds based on *in vitro* and *in silico* screening and profiling supported by its own know-how in chemistry, biology, bioinformatics and drug discovery. The leads are searched among the active compounds protected by BioZyne's European patent - EP0877022B1 and newly designed compounds are prepared using the know-how and technologies of the BioZyne research team. In 2012, several new families of compounds with promising in vitro anticancer activity were synthesized and tested. Their patent protection is under way.

EDUCATION

Members of the Division provided significant contributions to higher education by providing numerous courses at the undergraduate and graduate levels at the Universities of Zagreb, Rijeka, Osijek, Split and Dubrovnik. Members of DOCB are involved in several PhD programs, in particular, Chemistry – PhD program at the Faculty of Science, University of Zagreb, Medicinal Chemistry – PhD program at the Department of Biotechnology, University of Rijeka, Chemistry of Mediterranean Environment – PhD program at the University of Split, and Interdisciplinary Study in Molecular Biosciences (MOBI) − PhD program at Ruđer Bošković Institute, University of Osijek and University of Dubrovnik.

AWARDS

1. Marija Abramić received the RBI Annual Award for paper published in a journal with high impact factor.
2. Nikola Basarić received the RBI Annual Award for paper published in a journal with high impact factor.
3. Borislav Kovačević received the RBI Annual

Award for paper published in a journal with high impact factor.
4. Janja Makarević received the RBI Annual Award for paper published in a journal with high impact factor.
5. Mirjana Maksić received the RBI Annual Award for paper published in a journal with high impact factor.
6. Vjekoslav Štrukil received the RBI Annual Award for paper published in a journal with high impact factor.
7. Mario Vazdar received the RBI Annual Award for paper published in a journal with high impact factor
8. Robert Vianello received the RBI Annual Award for paper published in a journal with high impact factor.
9. Ivanka Jerić received the RBI Annual Award for an approved patent.
10. Davor Margetić received the RBI Annual Award for a published book.
11. Robert Vianello received the "Marie Curie Success Story" award for recognizing the results of his individual FP7 Marie Curie fellowship in the European Commissions's publication "EU FP7 People Specific Programme Success Stories Booklet."

PROJECTS

Programs supported by the Ministry of Science, Education and Sport

1. New small molecules targeting macromolecules of tumor and inflammatory processes, No: 0982914, Ivo Piantanida
2. Design, synthesis and reactivity of (bio)organic molecular systems, No: 0982933, Mirjana Maksić

Projects supported by the Ministry of Science, Education and Sport

1. Chiral building blocks for biological active molecules. Synthesis and reactivity; Zdenko Hameršak
2. Chiral organic materials - synthetic, structural and functional research; Vladimir Vinković
3. Cage compounds: building blocks for molecular architecture; Kata Majerski
4. Self-assembly in gels and synthesis of functional hybrid materials; Mladen Žinić
5. Synthesis of novel biologically active nucleobase and nucleotide derivatives; Biserka Žinić
6. Chemical transformations of natural compounds; Lidija Varga-Defterdarović
7. Molecular enzymology and protein interactions of hydrolases; Marija Abramić
8. 'Host-guest' interactions in polycyclic systems; Davor Margetić
9. Organic and bioorganic processes in ground and electronically excited states; Mirjana Maksić
10. Macrocyclic ligands, structures in solutions and molecular spectroscopies; Goran Baranović
11. Design, synthesis and study of interactions of small molecules with DNA, RNA and proteins; Ivo Piantanida
12. Brönsted and Lewis acids and bases in chemistry and biochemistry; Zvonimir Maksić/Robert Vianello
13. Computational studies of protein structure and function; David Smith

Research, developmental and international projects

1. Photochemistry of polycyclic molecules: From mechanistic studies to new drugs and medicinal applications. Nikola Basarić, HrZZ, No: 02.05/25.
2. Artificial Receptors for Bacillus anthracis Specific Anthrose Detection. Andreja Jakas and Predrag Cudic, NATO Science for Peace and Security Programme, No: CBP.EAP.SFP.983154.
3. Mechanochemistry for the clean and efficient metal-catalysed synthesis of pharmaceutical targets and the study of their molecular recognition. Mirjana Maksić, Unity Through Knowledge Fund, Croatia. Project type 1B, No: 63/10.
4. Computational Studies of Proton Dynamics in Hydrogen Bonded Systems and Enzymes (CoSProDyn), Robert Vianello, Individual

Intra-European Marie Curie Fellowship for Career Development, FP7–PEOPLE–2009–IEF call, No: FP7–255038.

5. Diversity in metallopeptidase family M49. Marija Abramić, Bilateral project Croatia-Austria.
6. Synthesis and spectroscopic study of anion fluorescence sensors. Nikola Basarić and Wenwu Qin, International Cooperation Project of the Natural Science Foundation of the Gansu Province, Bilateral project Croatia-China.
7. Semi-rational design of halohydrin dehalogenase HheA for application in the synthesis of chiral building blocks. Maja Majerić Elenkov, Bilateral project Croatia - P.R. China.
8. Design and synthesis of novel chiral cationic perylene bisimides and study of their interactions with DNA/RNA. Ivo Piantanida, Bilateral project DAAD Croatia-Germany.
9. Interactions of small organic molecules with nucleic acids: Synthesis, structural features and thermodynamics. Ivo Piantanida, Bilateral project Croatia-Slovenia.
10. Photoactive nano-structured gel systems with controlled optical properties, COGITO. Mladen Žinić and Jean-Luc Pozzo, Bilateral project Croatia-France.

SELECTED INVITED LECTURES

1. Vianello, Robert. Computational study of vibrational properties of histamine monocation: from aqueous solution to receptors. Jožef Stefan Institute, Ljubljana, Slovenia, February 29, 2012.
2. Majerski, Kata. The anion recognition through hydrogen bonding by adamantane-dipyrromethane receptors. School of Chemistry, University of KwaZulu-Natal, Durban, South Africa, March 6, 2012.
3. Eckert-Maksić, Mirjana. Guanidines - from theory to synthesis and applications. Sapienza-Università di Roma, Rome, Italy, March 22, 2012.
4. Majerski, Kata. Adamantane-(aminophenyl) dipirromethanes, bifunctional optical anion sensors. Polish Academy of Science, Institute of Physical Chemistry, Warsaw, Poland, April 12, 2012.
5. Vianello, Robert. 10 most important molecules of the 20th century. Science Festival, Rijeka, Croatia, April 26, 2012.
6. Vianello, Robert. Computational insight into the catalytic activity and the inhibition of monoamine oxidase B. 15th Amine Oxidase Conference, Toulouse, France, July 15 – 18, 2012.
7. Basarić, Nikola. Photochemical formation of quinone methides and investigation of their antiproliferative effect. EuCheMs, Organic chemistry division, 4th Young Investigators Workshop, Vienna, Austria, August 23 − 26, 2012.
8. Vianello, Robert. How are biogenic amines metabolized by monoamine oxidases? COST CM1103 Action Meeting "Structure-based drug design for diagnosis and treatment of neurological diseases: Dissecting and modulating complex function in the monoaminergic systems of the brain", Madrid, Spain, November 24 – 26, 2012.

SELECTED ORGANIZED CONFERENCES

1. Ruđer Josip Bošković Physicist and Astronomer, Symposium, Zagreb, May 25, 2011 (organizer Mirjana Maksić)

SELECTED PUBLICATIONS

1. Wu J, Zou Y, Sicking W, Piantanida I, Yi T, Schmuck C. A molecular peptide beacon for the ratiometric sensing of nucleic acids. *J Am Chem Soc* **134** (2012) 1958.
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Wernersson E, Heyda J, Jungwirth P. Overcharging in biological systems: reversal of electrophoretic mobility of aqueous polyaspartate by multivalent cations. *Phys Rev Lett* **108** (2012) 186101.

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6. Vazdar M, Pluhařová E, Mason P, Vácha R, Jungwirth P. Ions at hydrophobic aqueous interfaces: molecular dynamics with effective polarization. *J Phys Chem Lett* **3** (2012) 2087.
7. Štrukil V, Margetić D, Igrc MD, Eckert-Maksić M, Friščić T. Desymmetrisation of aromatic diamines and synthesis of non-symmetrical thiourea derivatives by click-mechanochemistry. *Chem Commun* **48** (2012) 9705.
8. Štrukil V, Igrc MD, Eckert-Maksić M, Friščić T. Click mechanochemistry: quantitative synthesis of "ready to use" chiral organocatalysts by efficient two-fold thiourea coupling to vicinal diamines. *Chem Eur J* **18** (2012) 8464.
9. Borštnar R, Repič M, Kamerlin SCL, Vianello R, Mavri J. Computational study of the pK_a values of potential catalytic residues in the active site of monoamine oxidase B. *J Chem Theory Comput* **8** (2012) 3864.
10. Horvat G, Stilinović V, Hrenar T, Kaitner B, Frkanec L, Tomišić V. An integrated approach (thermodynamic, structural and computational) to the study of complexation of alkali-metal cations by a lower-rim calix[4]arene amide derivative in acetonitrile. *Inorg Chem* **51** (2012) 6264.
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13. Vianello R, Repič M, Mavri J. How are biogenic amines metabolized by monoamine oxidases? *Eur J Org Chem* **2012** (2012) 7057.
14. Štrukil V, Igrc MD, Fábián L, Eckert-Maksić M, Childs SL, Reid DG, Duer MJ, Halasz I, Mottillo C, Friščić T. A model for a solvent-free synthetic organic research laboratory: click-mechanosynthesis and structural characterization of thioureas without bulk solvents. *Green Chem* **14** (2012) 2462.
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16. Štrukil V, Bartolec B, Portada T, Đilović I, Halasz I, Margetić D. One-pot mechanosynthesis of aromatic amides and dipeptides from carboxylic acids and amines. *Chem Commun* **48** (2012) 12100.
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18. Tumir L-M, Crnolatac I, Deligeorgiev T, Vasilev A, Kaloyanova S, Grabar Branilović M, Tomić S, Piantanida I. Kinetic differentiation between homo- and alternating AT-DNA by sterically restricted phosphonium dyes. *Chem Eur J* **18** (2012) 3859.
19. Veljković J, Uzelac L, Molčanov K, Mlinarić-Majerski K, Kralj M, Wan P, Basarić N. Sterically congested adamantylnaphthalene quinone methides. *J Org Chem* **77** (2012) 4596.
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23. Saftić D, Žinić B, Višnjevac A. DBU induced formation of 8-bromoguanosine dimer with three hydrogen bonds between the GG – base pairs. *Tetrahedron* **68** (2012) 1062.
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REVIEW ARTICLES

1. Maksić ZB, Kovačević B, Vianello R. Advances in determining the absolute proton affinities of neutral organic molecules in the gas phase and their interpretation: a theoretical account. *Chem Rev* **112** (2012) 5240.

CHAPTERS IN BOOKS

1. Barbatti M, Ruckenbauer M, Szymczak JJ, Sellner B, Vazdar M, Antol I, Eckert-Maksić M, Lischka H. Model systems for dynamics of pi-conjugated biomolecules in excited states. Handbook of Computational Chemistry, Leszczynski J (Ed.), Berlin Heidelberg, Springer-Verlag, 2012, 1175 − 1213.
2. Margetić D, Briš A. Microwave assisted furan cycloadditions: quantum-chemical reactivity assessment. Advances in Chemistry Research, Volume 15, Chapter 16, Taylor JC (Ed.), Nova Science Publishers, Inc., New York, 2012, 104 − 120.
3. Jakas A, Cudic P, Bionda N, Sućˇ J, Vlahoviček-Kahlina K, Cudic M. Peptide based artificial receptors for carbohydrate anthrose detection. Peptides 2012., Proc.32nd Eur. Peptide Symp. Kokotos G, Constantinou-Kokotou V, Matsoukas J. (Eds.), Athens, Greece, 2012, 314 − 315.

BOOKS

1. Margetić, Davor. Microwave assisted cycloaddition reactions, Chemical engineering methods and technology series, Nova Science Publishers, Inc., New York, 2011.

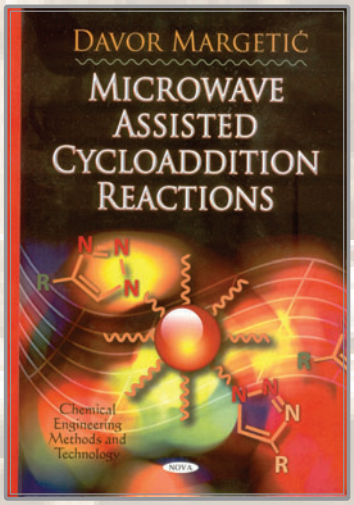


Fig. 13. Cover page of the book entitled Microwave assisted cycloaddition reactions.

Division of Materials Chemistry

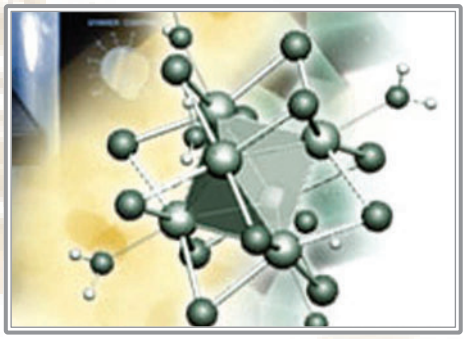
http://www.irb.hr/en/str/zkm

DIVISIONAL ORGANISATION

Head: Mira Ristić untill November (untill November 7), Damir Kralj

The Division of Materials Chemistry (ZKM) consits of the following laboratories:

- Laboratory for synthesis of new materials, Marijan Gotić
- Laboratory for precipitation processes, Damir Kralj
- Laboratory for radiation chemistry and dosimetry, Branka Mihaljević
- Laboratory for solid state and complex compounds chemistry, Antun Drašner
- Laboratory for ichtiopathology – biological materials, Rozelindra Čož-Rakovac



OVERVIEW OF THE DIVISION

In 2012 scientists in the Division of Materials Chemistry conducted basic and applied research on the synthesis, characterization and applications of different classes of materials, such as metal oxides, glass-ceramics, zeolites, slightly soluble ionic salts, cluster compounds, organic polymers, intermetalic compounds or metal hydrides. The physicochemical effects of ionizing radiation, its interactions with materials and development of chemical dosimetry systems were also studied. In addition, different terrestrial or aquatic organisms were used as biomodels / biosensors for genotoxic impact of nanomaterials at the subcellular, cell, tissue or organ level. Members of the Division participated in educational programs at the Universities of Zagreb, Osijek, Dubrovnik and Rijeka, conducting 17 undergraduate and postgraduate courses.

TOP ACHIEVEMENTS

Formation and properties of nickel oxide films and Ni/NiO nanocomposites

Differences in the formation and microstructures of NiO films formed on Ni plate or glass substrates were found. NiO particle sizes of films formed on Ni plates increased from nano to micro with the rise of heating temperature while the formation of NiO nanoparticles on glass substrates in the broad temperature range from 400 to 800 ^{o}C was explained by the absence of a constant source of metallic nickel which was present in the case of Ni plates (Marciuš et al., Alloys and Comp. 2012). A strong magnetic coupling between Ni (ferromagnetic) and NiO (antiferromagnetic) nanoparticles and grain-surface relaxations in Ni/NiO nanocomposites were found and explained by size and composition effects (Kremenović et al., 2012).

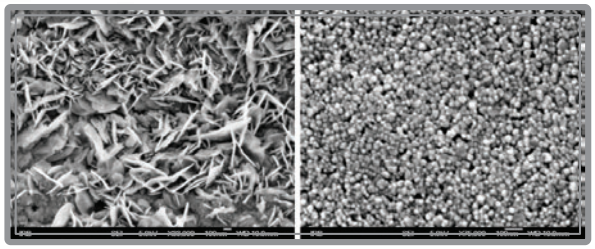


Fig. 1. NiO films nanostructures formed on different substrates: a) Ni plate (500 °C) and b) glass substrate (800 °C).

Lipidomics

The study of oxidative radical initiated-modifications of lipids or lipid peroxidation processes in model systems such as micelles and vesicles is motivated by aspects of the adverse consequences associated with peroxidation of unsaturated lipids in different natural and biological systems. A simple model system, suitable for the selective study of the lipid peroxidation propagation phase induced by ferrous was systematically presented. (Mihaljević et al., 2012).

Irradiation study of poly(ethylene oxide) in the solid state, melt and aqueous solution

The radiation outcome of poly(ethylene oxide), PEO, depended mostly on the aggregate state and on γ-irradiation conditions (total dose, atmosphere). Interactions of all influencing factors determined the thermal and crystalline properties of PEO as a polymer material for hydrogels and polyelectrolytes. (Jurkin et al., 2012).

DFT study of $CaNi_5H_x$ compounds **(0.0 ≤ x ≤ 1.0)**

Density functional theory based electronic structure calculations which included crystal structure optimizations were performed for CaNi5Hx (x=0.0,0.25,0.5,1.0) compounds. It was found that hydrogen atoms prefer, in notation of space group *P6/mmm*, 12n sites and that 3f sites are the second most preferred sites. The enthalpy of formation of α solid solution and for α ↔ β reaction was calculated.

Supramolecular architectures of novel chromium(III) oxalate complexes

A series of five novel compounds comprising the mononuclear $[Cr(L)_2(C_2O_4)]^+$ cations and/or the mononuclear $[Cr(L)(C_2O_4)_2]$ anions (L = 1,10-phenanthroline, 2,2'-bipyridine) were prepared and studied by crystallographic and spectroscopic methods. Steric effects of ligand size were studied as well as the complexing ability of the building blocks $[Cr(L)(C_2O_4)_2]^-$ in reaction with calcium(II) ions, resulting in new heterobimetallic polymeric compounds (Androš et al., 2012).

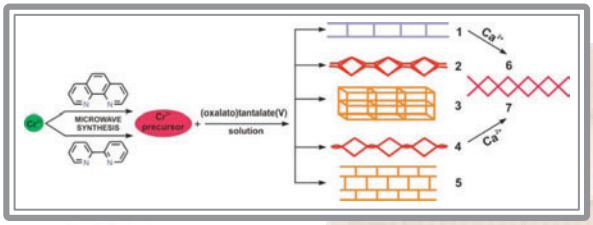


Fig. 2. Five new discrete chromium(III) oxalate complexes with overall two- (1, 2, 4, 5) or threedimensional (3) supramolecular architectures. Compounds 1 and 4 served as building blocks for the construction of heterobimetallic polymeric species (6, 7).

Backdoor induction

Amino acid substituted monodentate triphenylphosphines have been used as ligands in Rh(I) catalyzed asymmetric hydrogenation. Selectivity is induced by transmission of chirality *via* distant hydrogen-bonded amino acids with a *Herrick*-like secondary structure (Kokan and Kirin, RSC Adv. 2, 2012).

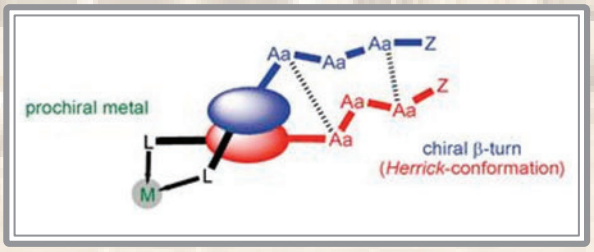


Fig. 3. Supramolecular bioinspired Rh(I) catalysts applied to asymmetric hydrogenation.

Fatty acid and proximate composition of bluefin tuna (Thunnus thynnus) muscle with regard to plasma lipids

The fatty acid and proximate composition of ventral ordinary tail muscle of Atlantic bluefin tuna, both farmed and wild was identified and this data compared with plasma parameters of farmed bluefin. The measured biochemical parameters were an excellent indicator of the overall metabolic equilibrium in bluefin tuna farmed for human consumption, which differed from wild specimens only in energy value, while significant differences were observable in their fatty acid profiles (Topić Popović et al., Aquaculture Research, 2012).

Unusual Pathway of Crystallization of Zeolite ZSM-5 in a Heterogeneous System: Phenomenology and Starting Considerations

The synthesis of high- and low-silica zeolites was described using several proposed mechanisms based on the chemical composition of the starting gel. New starting considerations are proposed which can explain the observed phenomena at the molecular level, before and during nuclei formation. (Ren *et al.*, 2012).

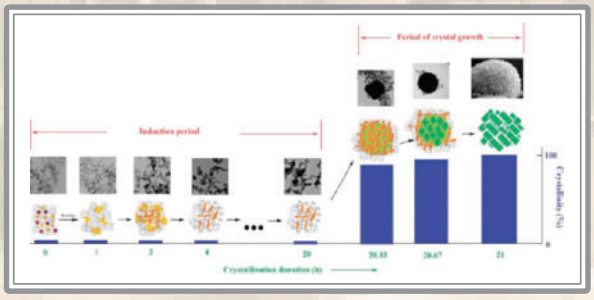


Fig. 4. Schematic Presentation of the Processes Occurring during Crystallization of ZSM-5.

Anomalous nucleation events during crystallization of zeolite A under marginal alkalinities: A population balance analysis

The processes of nucleation and crystal growth during crystallization in high and medium alkaline systems ($0.0165 \leq A \leq 0.046$) takes place in accordance with previously described experimental evidence. The anomalous kinetics of nucleation during crystallization of zeolite A from relatively low alkaline systems ($A \leq 0.01$) was not predicted theoretically nor found experimentally, until our recently published results (Bosnar *et al*., 2012).

Structural reorganization of acidic macromolecules during the calcium carbonate biomineralization

The growth of mineralized tissues during biomineralization is a biologically controlled process in which specific macromolecules are involved. Protein fragments containing a fluorescent tag were extracted from the green sheet of the abalone shell and were used as a probe to study changes in molecular structure during the precipitation of calcium carbonate polymorph(s). The obtained results indicated that conformational changes of a protein fragment occurred on moving from the solution to the mineral phase (Adamiano *et al*., 2012).

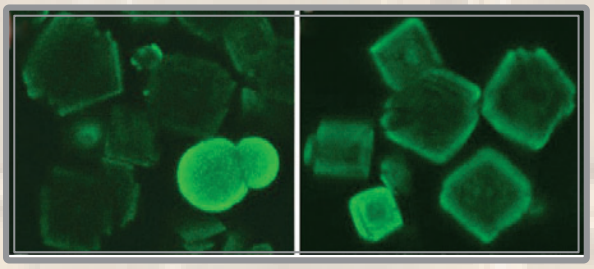


Fig. 5. Confocal laser scanning micrographs of calcium carbonate crystals precipitated in systems of lower and higher supersaturation and in the presence of fluorescing green layer peptide extracted from abalone shell.

NEW EQUIPMENT

Shaker mill Spex 8000M

EDUCATION

In 2012, scientists and researchers from the Division contributed to the educational programs at the Universities in Zagreb, Osijek, Dubrovnik and Rijeka, conducting 17 undergraduate and postgraduate courses and supervising 4 PhD theses.

AWARDS

Ruđer Bošković Institute Director's Annual Award (2012) for articles published in top scientific journals was given to Marijana Jurić, Goran Štefanić, Branka Njegić Džakula and Josip Bronić.

PROJECTS

Programs supported by the Ministry of Science, Education and Sports

1. New Functional Materials, Svetozar Musić

Projects supported by the Ministry of Science, Education and Sport

1. Synthesis and microstructure of metal oxides and oxide glasses, Mira Ristić
2. Study of influence of aluminosilicate precursors on their transformation, Josip Bronić
3. Precipitation mechanism of inorganic biocompatible and related materials, Damir Kralj
4. Metal hydrides in clean energy systems, Antun Drašner
5. Polynuclear metal systems – synthesis and properties, Berislav Perić
6. Structure-property relationships of modified polymer materials, Ivan Šmit
7. Physico-chemical effects of ionizing radiation in materials, Branka Mihaljević
8. Subcellular, biochemical and phylogenetic diversity of aquatic organisms, Rozelindra Čoz-Rakovac

Research, developmental and international projects

1. Investigations of factors influencing the properties of metallic and metal oxide nanoparticles. Mira Ristić (Croatian-Austrian bilateral scientific cooperation programme 2012-2013).
2. The influence of metal properties on nanoparticle-cell-interaction: cellular effects induced by noble metalnanoparticles. Marijan Gotić (Croatian-German bilateral scientific cooperation programme 2012-2013).
3. Biomimetic Radical Chemistry. Branka Mihaljević (Working group within COST CM1201).
4. European Radiation Dosimetry Group (EURADOS), Working group 3,6,9,12 within, Željka Knežević, Marija Majer, Saveta Miljanić, Maria Komor Ranogajec.
5. Japan-Croatian Agreement of Collaborative Research. Project coordinator Željka Knežević (Chiyoda Technol. Corporation & Ruđer Bošković Institute).
6. Enhancing quality control methods and procedures for radiation technology. Saveta Miljanić (IAEA Regional Technical Co-operation Project RER 8/017).
7. Introducing and harmonizing standardized quality control procedures for radiation technologies. Saveta Miljanić (IAEA Regional Technical Co-operation Project RER/1/011).
8. Enhancing the characterization, preservation and protection of cultural heritage artifacts. Irina Pucić (IAEA RER/0/034).
9. Passive solid state dosimetry systems - characterisation and application. Maria Komor Ranogajec (International project of the Croatian Academy of Sciences and Arts within agreement of scientific co-operation, Ruđer Bošković Institute and Institute of Isotopes and Hungarian Academy of Sciences).
10. Nuclear Techniques for the Characterization and Preservation of Cultural Heritage Artefacts. Branka Katusin Ražem (International project of the Croatian Academy of Sciences and Arts within agreement of scientific co-operation, Ruđer Bošković Institute, Institute

of Isotopes and Hungarian Academy of Sciences).

11. The effects of high-energy radiation on polymeric systems. Irina Pucić (International project of the Croatian Academy of Sciences and Arts within agreemnet of scientific co-operation, Ruđer Bošković Institute, Institute of Isotopes and Hungarian Academy of Science).
12. The synthesis of metal-organic framework materials for gasses storage and separation, Josip Bronić (Croatian-Slovenian bilateral scientific cooperation project 2012-2013).

SELECTED INVITED LECTURES

1. Gotić M: Wet-chemical synthesis of metal and metal oxides nanoparticles: 2nd Adriatic School of Nanoscience, ASON-2, Dubrovnik, Croatia, 2-7. September, 2012.
2. Topić Popović N: Antimicrobial drug resistance. 9th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 03, 2012.
3. Barišić J: Fatty acid composition of fish meat. 9th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 03, 2012.
4. Jadan M: Microsporidia – intracellular parasite and taxonomic nomad. 9th scientific-professional conference on autochthonous karstic species, Otočac, Croatia, June 03, 2012.
5. Knežević Ž: Evaluation of organ doses and radiation risk for CT examination of thorax: The 8th International Workshop on Ionizing Radiation Monitoring, Oarai, Japan, December 2, 2012.
6. Miljanić S: Radiotherapy out-of-field dosimetry: Clinical simulations of prostate radiotherapy using BOMAB-like phantoms, The 8th International Workshop on Ionizing Radiation Monitoring, Oarai, Japan, December 2, 2012.
7. Šmit I: X-ray diffraction of polymers: A short course on polymer characterization. POLYCHAR 20, Dubrovnik, Hrvatska, March 26, 2012.
8. Kirin S I: The application of “backdoor induction” in bioinspired asymmetric catalysis, NATO Advanced Research Workshop: Multidisciplinary Endeavour in Nanobiology, Nanoscience and Environment, Split, Croatia, April 16-20, 2012.

SELECTED ORGANIZED CONFERENCES AND MEETINGS

1. 9th scientific-professional conference on autochthonous karstic species, Otočac, June 03, 2012.
2. Meeting of Working group 12 within EURADOS, Zagreb, Croatia, December 04-05, 2012.
3. Irradiation methods in cultural heritage protection, Seminar for teachers in treatment and wood processing, with Agency for Vocational Education and Adult Education, Zagreb, Croatia, November 16, 2012.

SELECTED PUBLICATIONS

1. Kremenović A, Jančar B, Ristić M, Vučinić-Vasić M, Rogan J, Pačevski A, Antić B. Exchange-bias and grain-surface Relaxations in nanostructured NiO/Ni Induced by a particle size reduction. *J. Phys. Chem. C* **116** (2012) 4356.
2. Li Y, Štefanić G, Rathousky J, Hayden O, Bein T, Fattakhova-Rohlfing D. Assembly of mesoporous indium tin oxide electrodes from nano-hydroxide building blocks. *Chemical Science* **3** (2012) 2367.
3. Malev O, Sauerborn Klobučar R, Fabbretti E, Trebše P. Comparative toxicity of imidacloprid and its transformation product 6-chloronicotinic acid to non-target aquatic organisms: microalgae Desmodesmus subspicatus and amphipod Gammarus fossarum. *Pesticide Biochemistry and Physiology* **104** 3 (2012) 178.
4. Ren N, Subotić B, Bronić J, Tang Y, Dutour Sikirić M, Mišić T, Svetličić T, Bosnar S,

Antonić Jelić T. Unusual Pathway of Crystallization of zeolite ZSM-5 in heterogeneous system: Phenomenology and starting considerations. *Chem. Mater.* **24** (2012) 1726.
5. Bosnar S, Bronić J, Antonić Jelić T, Subotić B. Anomalous nucleation events during crystallization of zeolite A under marginal alkalinities: A population balance analysis. *CrystEngComm* **14** (2012) 3069.
6. Ren N, Bronić J, Antonić Jelić T, Palčić A, Subotić B. Population balance analysis of seed-induced, SDA-free crystallization of sub-micrometer zeolite ZSM-5. *Cryst. Growth Des.* **12** (2012) 1736.
7. Mihaljević B, Tartaro I, Filipović-Vinceković N. Evaluation of a model system for the selective study of the lipid peroxidation process. *Eur. J. Lipid Sci. Technol*. **114** 11 (2012) 1292.
8. Jurkin T, Pucić I. Poly(ethylene oxide) irradiated in solid state, melt and aqueous solution - DSC and WAXD study. *Rad. Phys. Chem. (1993)*. **81** 9 (2012) 1303.
9. Androš L, Jurić M, Molčanov K, Planinić P. Supramolecular architectures of novel chromium(III) oxalate complexes: steric effects of the ligand size and building-blocks approach. *Dalton Trans*. **41** (2012) 14611.
10. Adamiano A, Bonacchi S, Calonghi N, Fabbri D, Falini G, Fermani S, Genovese D, Kralj D, Montalti M, Njegić Džakula B, Prodi L, Sartor G. Structural Changes in a Protein Fragment from Abalone Shell during the Precipitation of Calcium Carbonate. *Chemistry - A European Journal*, **18** (2012) 14367-14374.

CHAPTERS IN BOOKS

1. Garaj-Vrhovac V, Gajski G, Milković Đ, Ranogajec-Komor M, Miljanić S, Beck N, Knežević Ž, Gerić M (2012). Radiation exposure and protection in conventional pediatric radiology of thorax. Radiation exposure Sources, Impacts and Reduction Strategies**.** Balenović D, Stimac E (eds). New York, Nova Science Publisher, Inc., 2012. pp 43-74.
2. Despot R, Hasan M, Rapp A O, Brischke Ch, Humar M, Welzbacher Ch R, Ražem D (2012). Changes in Selected Properties of Wood Caused by Gamma Radiation*.* Gamma Radiation, Chapter 14. Adrović F. (ed.), Rijeka, Croatia: InTech open science / open minds, 2012. pp 281-304.
3. Afgan E, Chapman B, Jadan M, Franke V, Taylor J (2012). Using Cloud Computing Infrastructure with CloudBioLinux, CloudMan, and Galaxy. Current Protocols in Bioinformatics / Baxevanis, Andreas D. (ed). Marylend: Wiley, 2012. pp 11.9.1-11.9.20.
4. Ren N, Subotić B, Bronić J (2012). Crystallization of Sub-Micrometer Sized ZSM-5 Zeolites in SDA-Free Systems, in Advances in Crystallization Processes, Mastai, Yitzak (Ed.), Rijeka, In Tech, 2012. pp. 259-284.

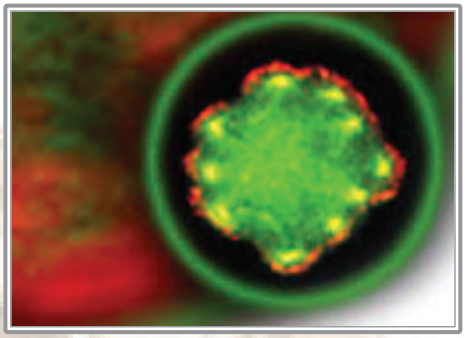
Division of Molecular Biology

DIVISIONAL ORGANISATION

Head: Igor Weber

The Division of Molecular Biology consists of the following laboratories:

- Laboratory of Neurochemistry and Molecular Neurobiology, Lipa Čičin-Šain
- Laboratory for Electron Microscopy, Hrvoje Fulgosi
- Laboratory for Genotoxic Agents, Maja Osmak
- Laboratory for Structure and Function of Heterochromatin, Miroslav Plohl
- Laboratory of Molecular and Cell Biology, Ivica Rubelj
- Laboratory of Chemical Biology, Branka Salopek Sondi
- Laboratory for Evolutionary Genetics, Đurđica Ugarković
- Laboratory for Molecular Genetics, Dušica Vujaklija
- Laboratory of Molecular Microbiology, Davor Zahradka



OVERVIEW OF THE DIVISION

The mission of the Division of Molecular Biology is to advance our knowledge on fundamental biological questions by conducting high-quality, internationally recognized knowledge-driven scientific research on major topics in contemporary biology, from molecules to cells and organisms. We also participate in knowledge transfer by contributing to education, and by offering expertise and application of acquired knowledge, methodologies and skills to the broader community. Research areas in the Division are focused on exploring different aspects of molecular and cellular biology studied on microbial, animal and plant organisms. Particular goals of the research program are to explore non-coding repetitive sequences in genome structuring; to study structures and processes at telomeres; to study processes essential for maintaining genome integrity, plasticity and evolution; to decipher evolutionary patterns of conserved genes and appearance of new genes; to characterize general and specific transcription factors and their mechanisms of action; to study how cells communicate, differentiate, move and adhere; to investigate molecular mechanisms involved in the cellular response to genotoxic compounds; to examine the potential of genetically targeted adenoviruses; to explore photosynthesis; and to study the role of bioactive molecules, plant hormones and secondary metabolites, in plant growth, development and stress response.

TOP ACHIEVEMENTS

Endogenous plant hormone auxin – the role in the Christmas rose flower development

The aim of this study was to evaluate the role of the plant hormone auxin originating in the developing seed on the post-anthesis flower development of the Christmas rose. This study suggests that auxin arising in developing fruit may participate, in part, in coordination of the Christmas rose peduncle elongation and its vascular development (Brcko et al. 2012).

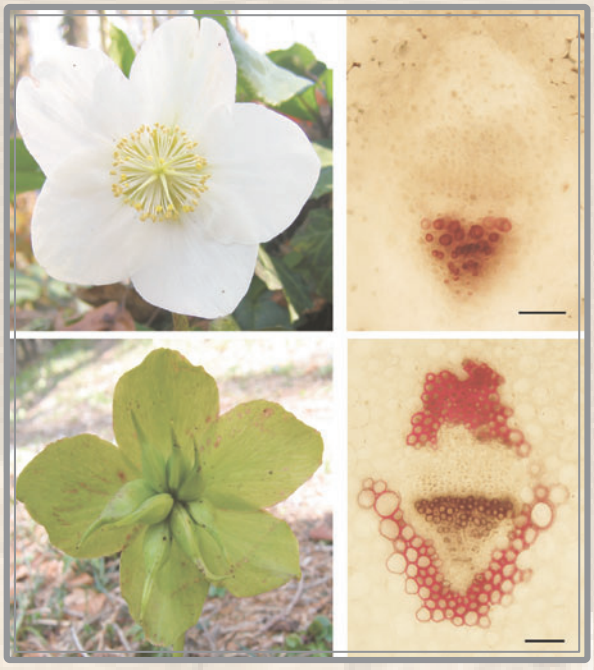


Fig. 1. Lignin accumulation (red) in the peduncle vascular tissue during the Christmas rose flower development: white flower before fertilization (upper part) and fruit bearing flower (lower part) with accompanying vascular bundles. Bars: 100 µm.

A dual role for Rac1 GTPases in the regulation of cell motility

Evidence is obtained through the use of specific fluorescently labeled probes that activated Rac1 GTPases are involved in regulation of actin cytoskeleton dynamics both at the front and the back of migrating *Dictyostelium* cells. This finding suggests a novel principle for regulation of Rho GTPase activity that might also play a role in other cell types and for other Rho family members (Filić et al., 2012).

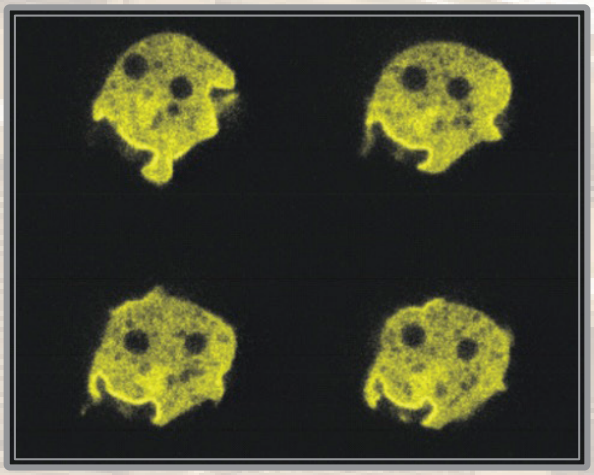


Fig. 2. Formation of a macropinocytotic cup in a Dictyostelium discoideum cell that expresses a fluorescent probe for activated Rac1 GTPases.

Oyster genome sequencing

Domazet-Lošo T participated in the pacific oyster genome study where he was involved in the analysis of developmental expression profiles. This study reflects international efforts to improve genomic resources for molluscs, an important animal phylum that contains many species relevant to the human diet (Zhang et al., 2012).

Evolution of stem cells

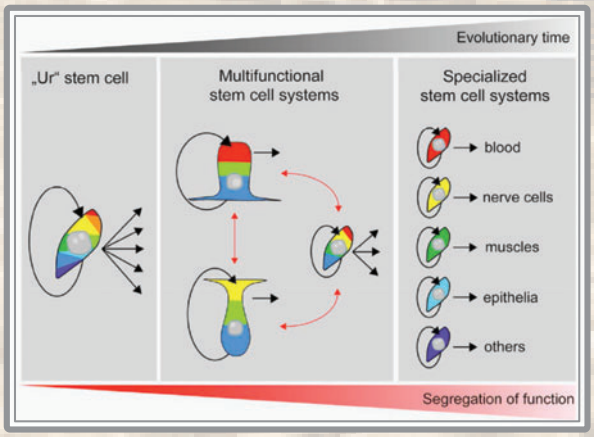


Fig. 3. Scenario for the evolution of metazoan complexity based on the diversification of stem cell systems.

Evolutionary origin of the stem cell system in animals has still not been fully resolved. This work shows that interstitial stem cells in Hydra express an evolutionary oldest transcriptome, suggesting that ancient stem cells were multifunctional (Hemmrich et al., 2012).

Degradation of chloroplast DNA at the onset of natural leaf senescence in trees

We determined that chloroplast DNA (cpDNA) starts to degrade at the onset of leaf yellowing in the maple. It appears that during all stages of leaf senescence proteinaceous components stay firmly bound to a region of cpDNA containing the gene rbcL, which encodes the large subunit of the enzyme RUBISCO, which might be important for the down-regulation of rbcL expression during natural leaf senescence (Fulgosi et al., 2012).

Interplay of helicases and nucleases in the RecF recombinational pathway

The role of RecQ, UvrD and HelD helicases in the initiation stage of the RecF recombinational pathway in *E. coli* has been examined. The results suggest (i) that a significant portion of recombination events in the RecF pathway is independent of RecQ, UvrD and HelD, and (ii) that elimination of nucleases acting on 3' ssDNA ends reduces the necessity for helicases in the initiation of recombination (Buljubašić et al., 2012)

Satellite DNA and stress response

Satellite DNA-associated siRNAs are transiently activated after heat shock and affect epigenetic state of constitutive heterochromatin in beetle *Tribolium castaneum*. It is proposed that transient remodeling of heterochromatin is part of a physiological gene expression program activated under stress conditions in insects (Pezer and Ugarković, 2012).

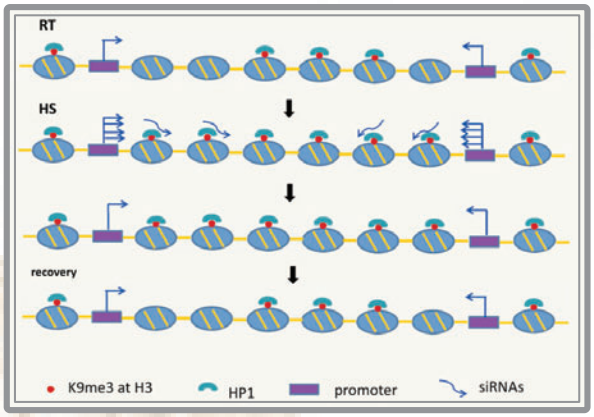


Fig. 4. The proposed negative-feedback mechanism of epigenetic changes in heterochromatin induced by heat stress. Satellite RNAs induced after heat stress repress their own transcription by providing additional histone3 lysin9 me3 (H3K9me3) anchorage sites for the chromodomain protein such as HP1.

Ikaros family transcription factor expression in rat thymus: detection of impaired development

The data presented in this paper show for the first time mRNA expression of Ikaros family transcription factors Ikaros, Aiolos, Helios and Pegasus (Paradžik et al., 2012).

Structural and functional characterization of ribosomal protein gene introns in sponges

Ribosomal protein genes (RPGs) are a powerful tool for studying intron evolution. Our results show that sponge RPG introns, although very dynamic, share many structural characteristics with "higher" metazoans. These similarities are probably important because RPG introns function as carriers of snoRNAs, essential elements for ribosome assembly (Perina et al., 2012).

DNA end resection controls the balance between homologous and illegitimate recombination

Even a partial loss of function of the conserved human RecQ helicase analogs causes adverse effects such as cancer-

prone Werner, Bloom or Rothmund-Thompson syndrome, whereas a complete RecQ deficiency in *E. coli* is not deleterious for the cell. We show that this puzzling difference is due to different mechanisms of DNA double strand break (DSB) resection in *E. coli* and humans (Ivanković and Đermić, 2012).

EDUCATION

In 2012, members of the Division of molecular biology participated in the teaching of more than 15 undergraduate and graduate courses and more than 20 postgraduate at the Universities in Zagreb, Split, Dubrovnik and Osijek. In addition, they supervised more than 15 diploma, MSc, and PhD theses. A series of practical courses in biology and medicine was organized in our Division by Andreja Ambriović Ristov (http://www.tecajevi-irb.com).

AWARDS

Maja Osmak, Tamara Čimbora-Zovko and Anamaria Brozović received the Annual RBI award for an internationally accepted patent.

Hrvoje Fulgosi, Damir Đermić, Dragutin Perina, Marina Korolija, Andreja Mikoč, Bruna Pleše, Mirna Imešek, Renato Batel and Helena Ćetković received the Annual RBI award for scientific publication.

Mariastefania Antica received the Annual RBI award as book editor.

PROJECTS

Program supported by the Ministry of Science, Education and Sport

1. Molecular fundaments of biological processes, Miroslav Plohl.

Projects supported by the Ministry of Science, Education and Sport

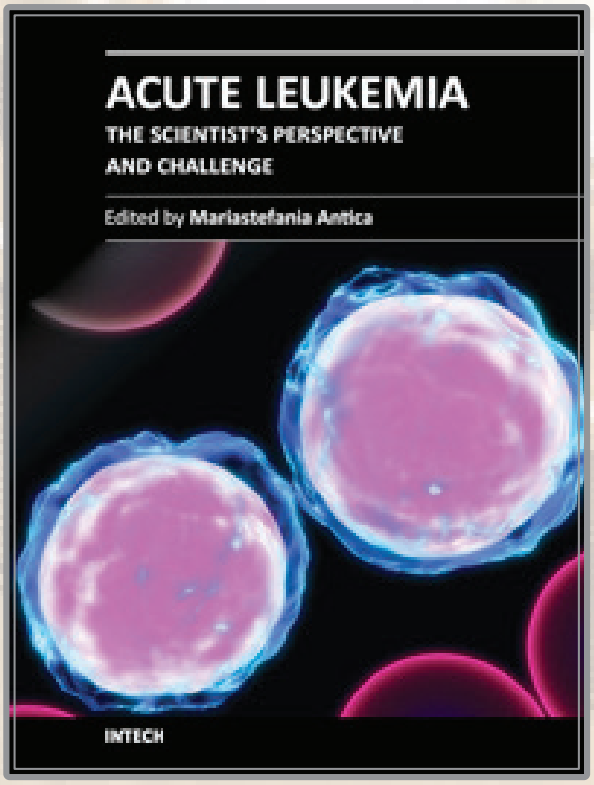


Fig. 5. This book provides a comprehensive overview of the basic mechanisms underlying acute leukemia, current advances, and future directions in management of this disease.

1. Increase of adenovirus transduction efficacy and resistance to cytostatics, Andreja Ambriović Ristov
2. Molecular interactions in lymphocyte differentiation, Mariastefania Antica
3. The role of recombination in DNA repair and genome evolution, Krunoslav Brčić-Kostić
4. Genes and genomes: structure, function and evolution, Helena Ćetković
5. Serotonergic mechanisms in alcoholism, Lipa Čičin-Šain
6. Genetic studies of BPC-157 effect on microorganisms, Senka Džidić
7. Regulatory mechanisms of photosynthesis and differentiation of plastids, Hrvoje Fulgosi
8. Hydrodynamics of cerebrospinal fluid, Darko Orešković
9. Cell response to cytotoxic agents and resistance development, Maja Osmak
10. Evolution, properties and functional interactions of satellite DNA sequences, Miroslav Plohl

11. Molecular mechanisms of immortalization and cellular aging, Ivica Rubelj
12. Molecular regulation of plant development, Branka Salopek-Sondi
13. Transcriptional regulation in eukaryotes, Mary Sopta
14. Serotonergic transmission: genes, proteins and behavior, Jasminka Štefulj
15. Evolution and function of fast evolving portion of eukaryotic genome, Đurđica Ugarković
16. Fundamental molecular studies of Streptomyces biology, Dušica Vujaklija
17. Regulation of the cytoskeleton dynamics in cell motility and cytokinesis, Igor Weber
18. Molecular mechanisms of DNA recombination and repair, Davor Zahradka

Research, developmental and international projects

1. Dissecting complex regulators of photosynthetic energy conversion, Hrvoje Fulgosi (International Center for Genetic Engineering and Biotechnology, CRP/CRO11-01)
2. EpiGeneSys, WP4: Signalling to the Epigenome, Đurđica Ugarković (EC FP7 Network of Excellence)
3. Construction, development and application of target vectors, Ivica Rubelj (Croatian Institute of Technology)
4. Identification of gene pathways involved in serotonergic modulation of body weight, Lipa Čičin-Šain (TANITA Healthy Weight Community Trust)
5. Transport of serotonin across placenta: studies on primary endothelial cells of human placental barrier, Jasminka Štefulj (MZOS, bilateral project with Austria, 910-08/11-01/00105)
6. Proteins linking photosynthesis with plant antioxidative responsens to stress, Hrvoje Fulgosi (MZOS, bilateral project with Austria, 910-08/11-01/00099)
7. Platinum compounds-induced stress responses and mechanimsm of resistance, Maja Osmak (MZOS, bilateral project with Germany, 910-08/11-01/00292)
8. Control of plant growth and senescence by energetic status of chloroplasts, Hrvoje Fulgosi (MZOS, bilateral project with Germany, 910-08/10-01/00192)
9. Diaryrtriazens: a new group of potential anticancer drugs, Anamaria Brozović (MZOS, bilateral project with Slovenia, 910-08/08-01/00312)
10. Epigenetics: Bench to Bedsite, Đurđica Ugarković (COST Action TD0905)
11. Development of DNA markers for identifying commercially important mollusk species Ruditapes decussatus in the Adriatic Sea, Brankica Mravinac (Adris Foundation)
12. Analyses of plant hormone auxin, salicylic acid and jasmonic acid in *Brassica rapa* L. var. *pekinesis* upon abiotic stress, Branka Salopek-Sondi (Croatian Academy of Sciences and Arts – HAZU)
13. Regenerative potential of stem cells and their microenvironment, Mariastefania Antica (Croatian Academy of Sciences and Arts – HAZU)
14. Authenticity of white cabbage cv. 'Varaždinski' evaluated by RAPD markers, Branka Salopek-Sondi (Varaždin County)

SELECTED INVITED LECTURES

1. Orešković D, Klarica M: Various perfusion methods in determination of CSF net formation and unidirectional flow. Hydrocephalus 2012 - 4th Meeting of the International Society of Hydrocephalus and CSF Disorder. Kyoto, Japan, October 19-22, 2012.
2. Ugarković Đ: Environmental stimuli induce remodelling of heterochromatin in insects. BIT's Second Annual World Congress of Molecular & Cell Biology. Beijing, China, May 17-20, 2012.
3. Bilandžija H: Convergent Evolution of Albinism in Diverse Cave Adapted Animals. 21st International Conference on Subterranean Biology. Košice, Slovačka, September 2-7, 2012.
4. Vujaklija D: A new look at SSB proteins. Symposium: Actinobacteria within soils-Capacities for mutualism, symbiosis and pathogenesis. Münster ,Germany, October 25-28, 2012.

5. Ugarković Đ: DNA demethylation and heterochromatin remodelling upon heat stress. COST action TD0905 Workshop. Salerno, Italy, November 4-6, 2012.
6. Meštrović N: Satellite DNAs library in the process of forming: the nematode view. 3rd Congress of Croatian Geneticists with international participation. Krk, Croatia, May **13-16**, 2012.
7. Weber I: Rac1 GTPases play a dual role in the regulation of cell motility. Croatian Microscopy Symposium. Pula, Croatia, November 16-17, 2012.
8. Vujaklija D: New insights into bacterial phosphoproteome analysis. Summer School on Microbial Metabolites in Nature and Medicine. Dubrovnik, Croatia, August 25-September 2, 2012.
9. Weber I: A dual role for Rac1 GTPases in the regulation of cell motility. Regional Biophysics Conference. Kladovo, Serbia, September 03-07, 2012.
10. Fulgosi H: Resolving electron partitioning in oxygenic photosynthesis. Science Society of Styria and the Institute of Plant Sciences, Karl-Franzens University. Graz, Austria, October 23, 2012.
11. Fulgosi H: Energy partitioning in photosynthesis - new modes of regulation. Biological Center, Christian-Albrechts-University. Kiel, Germany, June 20, 2012.
12. Vujaklija D: What is the biological role of paralogous SSBs in *Streptomyces coelicolor*? Université de Pau et des Pays de l'Adour, Equipe Environnement et Microbiologie. Pau, France, December 21, 2012.

SELECTED ORGANIZED CONFERENCES

1. 3rd Congress of Croatian Geneticists, Krk, Croatia, May 13-16, 2012 (D. Vujaklija)
2. 5th Croatian Congress of Microbiology with international participation, Primošten, Croatia, September 26-30, 2012 (D. Vujaklija)
3. 11th Croatian Biological Congress, Šibenik, Croatia, September 16-21, 2012 (H. Ćetković)

SELECTED PUBLICATIONS

1. Filić V, Marinović M, Faix J, Weber I. A dual role for Rac1 GTPases in the regulation of cell motility. *J Cell Sci* **125** (2012) 387.
2. Pezer Z, Ugarković Đ. Satellite DNA-associated siRNAs as mediators of heat shock response in insects. *RNA Biol* **9** (2012) 587.
3. Buljubašić M, Repar J, Zahradka K, Đermić D, Zahradka D. RecF recombination pathway in *Escherichia coli* cells lacking RecQ, UvrD and HelD helicases. *DNA Repair* **11** (2012) 419.
4. Perina D, Korolija M, Mikoč A, Roller M, Pleše B, Imešek M, Morrow C, Batel R, Ćetković H. Structural and functional characterization of ribosomal protein gene introns in sponges. *PLoS ONE* **7** (2012) e42523.
5. Ivanković S, Đermić D. DNA end resection controls the balance between homologous and illegitimate recombination in *Escherichia coli*. *PLoS ONE* **7** (2012) e39030.
6. Zhang G,..... Domazet-Lošo T,..... Wang J. The oyster genome reveals stress adaptation and complexity of shell formation. *Nature* **490** (2012) 49.
7. Brcko A, Penčik A, Magnus V, Prebeg T, Mlinarić S, Antunović J, Lepeduš H, Cesar V, Strnad M, Rolčik J, Salopek-Sondi B. Endogenous auxin profile in the Christmas rose *(Helleborus niger L.)* flower and fruit: Free and amide conjugated IAA. *J Plant Growth Regul* **31** (2012) 63.
8. Paradžik M, Novak S, Mokrović G, Bordukalo Nikšić T, Heckel D, Stipić J, Pavičić Baldani D, Čičin-Šain L, Antica M. Ikaros Family transcription factors expression in rat thymus: detection of impaired development. *Int J Immunopathol Pharmacol* **25** (2012) 893.
9. Hemmrich G, Khalturin K, Boehm AM, Puchert M, Anton-Erxleben F, Wittlieb J, Klostermeier UC, Rosenstiel P, Oberg HH, Domazet-Lošo T, Sugimoto T, Niwa H, Bosch TC. Molecular signatures of the three stem cell lineages in hydra and the emergence of stem cell function at the base of multicellularity. *Mol Biol Evol* **29** (2012) 3267.

10. Fulgosi H, Ježić M, Lepeduš H, Peharec Štefanić P, Ćurković Perica M, Cesar V. Degradation of chloroplast DNA during natural senscence of maple leaves. *Tree Physiol* **32** (2012) 346.
11. Ivanković M, Ćukušić Kalajžić A, Škrobot Vidaček N, Franić Šimić I, Davidović Mrsić S, Rubelj I. Human Xp/Yp telomere analysis by Southern-STELA. *Biogerontology* **13** (2012) 203.

Review articles

1. Osmak M. Statins and cancer: Current and future prospects. *Cancer Lett* **324** (2012) 1.

Chapters in books

1. Plohl M, Meštrović N, Mravinac B. Satellite DNA evolution. In: Repetitive DNA, Garrido-Ramos MA (ed), Basel, Karger AG, 2012. pp 126-152.
2. Pezer Ž, Brajković J, Feliciello I, Ugarković Đ. Satellite DNA-mediated effects on genome regulation. In: Repetitive DNA, Garrido-Ramos MA (ed), Basel, Karger AG, 2012. pp 153-169.
3. Vujaklija D, Maček B. Single-Stranded DNA binding proteins: Detecting Posttranslational Modificatios of Bacterial SSB Proteins. In: Springer Protocols, Keck JL (ed), New York, Humana Press, 2012. pp 205-218.
4. Vojta L, Fulgosi H. Energy conductance from thylakoid complexes to stromal reducing equivalents. In: Advances in Photosynthesis - Fundamental Aspects, Najafpour MM (ed), Rijeka, InTech, 2012.

BOOKS

1. Vojta L. Protein Import into Chloroplasts - From cytosolic translation to the final destination. Lambert Academic Publishing, Saarbrücken, 2012.

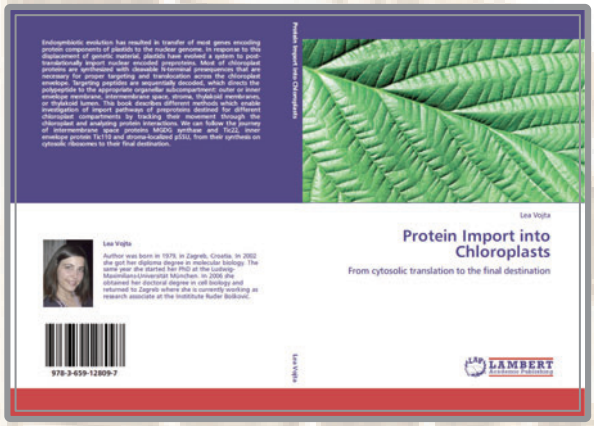


Fig. 6. This book describes different methods which enable investigation of import pathways of preproteins destined for different chloroplast compartments by tracking their movement through the chloroplast and analyzing protein interactions.

Division of Molecular Medicine

http://www.irb.hr/en/str/zmm

DIVISIONAL ORGANIZATION

Head: Oliver Vugrek, PhD (Previously: Đurđica Ugarković until Jan 29th, 2012, and Koraljka Gall-Trošelj from Jan 30th until May 30th, 2012).

The Division of Molecular Medicine (ZMM) consists of the following laboratories:

- Laboratory for Systems Biomedicine, Mario Cindrić
- Laboratory of Experimental Hematology, Immunology and Oncology, Jelka Gabrilovac
- Laboratory of Molecular Virology and Bacteriology, Magdalena Grce
- Laboratory of Molecular Endocrinology and Transplantation, Mirko Hadžija
- Laboratory of Experimental Therapy, Marijeta Kralj
- Laboratory for Reactive Radicals, Tatjana Marotti
- Laboratory of Molecular Neuropsychiatry, Dorotea Mück-Šeler
- Laboratory of Molecular Oncology, Jasminka Pavelić
- Laboratory for Epigenomics, Koraljka Gall Trošelj
- Laboratory of Molecular Neuropharmacology, Silva Katušić Hećimović
- Group for Translation Medicine, Oliver Vugrek
- Laboratory for Oxidative Stress, Neven Žarković
- Laboratory for Hereditary Cancer, Sonja Levanat
- Laboratory for Personalized Medicine, Sanja Kapitanović
- Animal Facility Unit, Ranko Stojković

OVERVIEW OF THE DIVISION

The mission of the DMM is further affirmation as a center of expertise and innovation to become a dynamic actor in the European Research Area (ERA), and to foster leadership in regional economic and socially sustainable development to overcome challenges to advanced health care for the benefit of actual and future patients.

DMM integrates molecular and cell biology, biochemistry, high-throughput technologies, bioinformatics, biostatistics, and engineering to derive predictive, quantitative models for biological systems. Aligned with disease based models and clinical research, DMM has the potential to steer medical research into new avenues of innovation and technology, and the next century of personalized medicine.

The Division of Molecular Medicine, with its numerous valuable samples collected through long-standing collaborations with clinicians (e.g. in oncology, neuroscience and others), represents an important biomedical core.

DMM engages in interdisciplinary research with a focus on deciphering the 'post-transcriptional regulatory code' and to

integrate it with other major cellular regulatory mechanisms, in particular signal transduction pathways, cell death regulation, protein-protein interaction networks, and post-translational modifications. To do so, several disease based models are available ranging from cancer, imprinting and methylation disorders, neurodegenerative diseases, and others. Accordingly, this serves as the basis for a global understanding of cellular processes in both health and disease and how they may be used to facilitate disease prevention, diagnosis and therapy.

Human resources, skills, and methodology, the key for taking DMM to the next level of biomedical research and science and technology are available in all mentioned fields. The necessary infrastructure for basic and applied biomedical research is present, and steadily improved through competitive grants. Towards that end, integrative efforts have been significantly boosted through success in negotiating European community funded grants implemented within the instrument for preaccession assistance (IPA). This indicates existing excellence in science and technology (S&T) within the ERA, and in particular in the health domain. Altogether, building on the expertise of present senior researchers, a large number of Early Stage Researchers (ESR) and State-of-the-Art infrastructure, the DMM provides all of the required building blocks to excel beyond State-of-the-Art.

TOP ACHIEVEMENTS

Acute fluvoxamine administration affects 5-HT synthesis rates in the rat brain regions

Using an autoradiographic method, we have found that the single administration of the serotonin (5-HT) uptake blocker, fluvoxamine, affected 5-HT synthesis rates throughout the brain. A significant (raphe magnus) and a trend (dorsal and median raphe) of decreased 5-HT synthesis rates in serotoninergic cell body areas, and increased (hippocampus, substantia nigra, hypothalamus) or unchanged (caudate-putamen, nucleus accumbens) 5-HT synthesis rates were found in the nerve terminal regions. These regional specific effects of fluvoxamine on 5-HT synthesis might be mediated by the presynaptic serotonergic autoreceptors (Muck-Šeler et al., 2012).

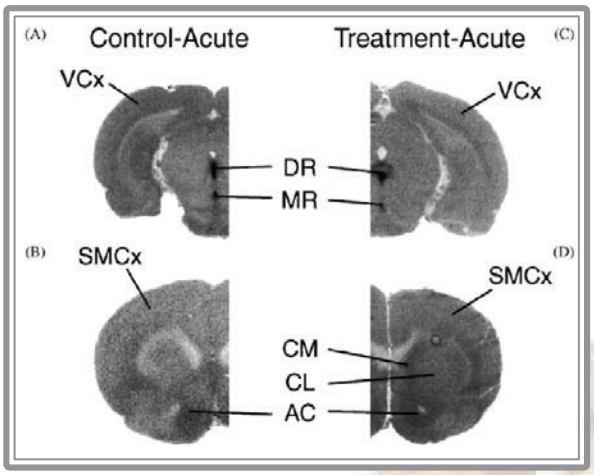


Figure 1. A set of representative autoradiograms obtained in rats used in the acute and 7-day treatments: control rats (A, B) and rats treated with fluvoxamine (25 mg/kg, i.p.; C, D). (AC, nucleus accumbens; CM, caudate-medial; CL, caudate-lateral; DR, dorsal raphe; MR, median raphe; P, pineal body; VCx, visual cortex; SMCx, sensory-motor cortex).

Add-on treatment with quetiapine improves depression, aggression, irritability and suicidal tendencies in children and adolescents

In a pilot trial, clinical improvement after 24 weeks of atypical antipsychotic quetiapine treatment, added to standard selective serotonin reuptake inhibitors (SSRIs), ameliorated aggressive behaviour, intentional self-injury, chronic anxiety and affective instability, depression, suicidal tendencies and irritability in children and adolescents with developing borderline personality disorder (Podobnik et al., 2012).

The effect of ziprasidone treatment on platelet 5-HT concentration in patients with schizophrenia

Ziprasidone is an atypical antipsychotic, whose antidepressant properties are presumably achieved via blockade of the serotonin transporter (5-HTT) and inhibition of synaptic serotonin (5-HT) reuptake. Platelet 5-HT concentration is a reliable marker of the 5-HTT blockade induced by SSRIs. We were the first to study the "in vivo" effects of ziprasidone, and have found that ziprasidone did not affect platelet 5-HT concentration in schizophrenic patients before, and after 7 and 28 days of treatment, suggesting that ziprasidone does not affect 5-HT reuptake "in vivo" (Šagud et al., 2012).

Aristolactam-DNA adducts as biomarkers of environmental exposure to aristolochic acid, causative agent of endemic nephropathy

Endemic (Balkan) nephropathy has been linked to exposure to aristolochic acid, a powerful nephrotoxin and human carcinogen. Following metabolic activation, aristolochic acid reacts with genomic DNA to form aristolactam-DNA adducts that generate a unique TP53 mutational spectrum in the urothelium. This paper presents the molecular epidemiologic evidence that strongly supports the hypothesis that, in genetically susceptible individuals, dietary exposure to aristolochic acid is causally related to endemic nephropathy and to carcinomas of the upper urinary tract associated with this disease (Jelaković et al., 2012)

Putative mechanisms of antitumor activity of cyano-substituted heteroaryles in HeLa cells

The antitumor mechanisms of action of cyano-substituted heteroaryles depend on the position of the cyano-group; while cyano-substituted naphthiophene reduced the expression of cytoskeletal proteins, cyano-substituted thieno-thiophene-carboxanilide inhibited the formation of cellular reactive oxygen species (Ester et al., 2012).

Novel HPV 16 variant

Whole genome analysis of a novel human papillomavirus (HPV) type 16 E1 variant, E1-1374^63nt , revealed several other mutations common to this variant, of which four were novel mutations, all within the E1 region. This variant is significantly more associated with lower grade cervical lesions in comparison to other HPV 16 variants and its determination should be considered in further epidemiology studies of HPV variants (Sabol et al. 2012).

New case of AHCY deficiency

The seventh known patient with S-adenosylhomocysteine hydrolase (AHCY) deficiency exhibiting a new allelic mutation has been identified. The case shows a unique disease pattern presented at birth with features resembling phosphomannomutase 2 (PMM2-CDG Ia) deficiency (Honzik et al., 2012). AHCY deficiency should be considered in early infancy when PMM2-CDG Ia deficiency is suspected but appropriate laboratory tests do not reveal altered glycosylation patterns.

Cholesterol levels modulate trafficking of the key proteins in Alzheimer's disease within endosomal-lysosomal pathway

Using a rare inherited disorder of cholesterol transport Niemann-Pick type C we have identified a cholesterol-dependent alterations of the trafficking within endosomal-lysosomal pathway of the two key proteins in Alzheimer's disease: amyloid precursor protein (APP) and beta-site APP cleaving enzyme 1 (BACE1) (Malnar et al. 2012). These findings may shed light on the molecular mechanisms of how increased cholesterol levels may trigger Alzheimer's disease.

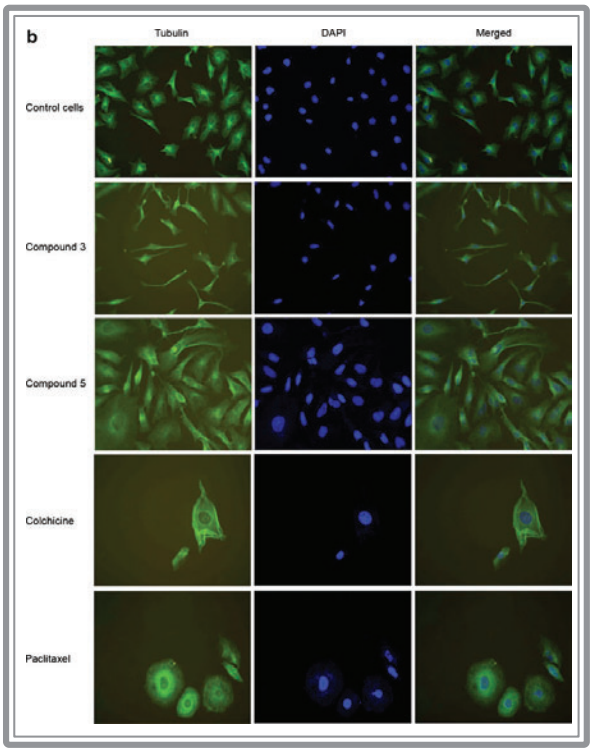


Figure 2. Cyano-substituted compounds perturb cytoskeleton. Cellular tubulin was stained using immunofluorescence, and positive controls included Paclitaxel and Colchicine. DAPI was used to stain nuclei.

NEW EQUIPMENT

Bioreactor

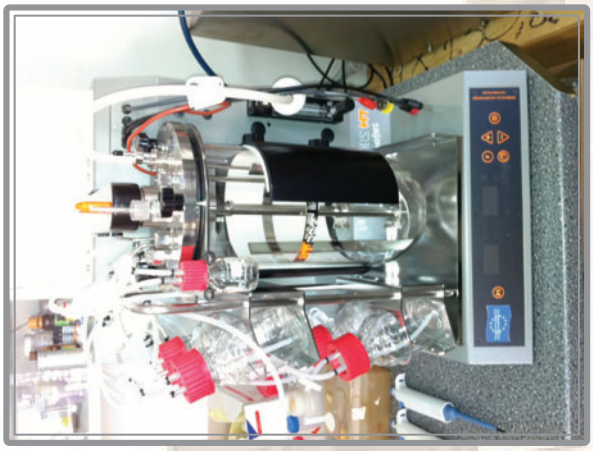


Fig 3. Phylogenic clustering of E1-1374ˆ63nt variant sequences with other currently available published HPV16 whole genome sequences and the whole genome sequences of four Croatian E1-1374ˆ63nt variant samples, ZG01-118, ZG01-258, ZG03-145 and ZG05-249 (Sabol et al. 2012).

The bioreactor is a starting point for fermentation in research and education and also a very cost-effective way to produce large amounts of recombinant proteins, and high densities of eukaryotic cell cultures for downstream applications, respectively. The bioreactor allows automated control of pH, CO2, O2, feeding, sampling and software for data-logging during operation.

Human ORFeome collection

The human ORFeome collection serves as an extremely efficient shortcut as almost every known human gene will be available for subsequent R&D activities. At present more than 13000 individual human full length cDNA clones are available at RBI. Due to the extreme simplification of the cloning processes by using the Gateway cloning system, the hORFeome enables cost effective subcloning of genes of interest into appropriate expression vectors for basic and applied research applications.

EDUCATION

DMM researchers were very active in education at different universities - University of Zagreb (Faculty of Science, School of Medicine, School of Pharmacy and Biochemistry, The Faculty of Veterinary Medicine, Academy of Art), University of Rijeka (Faculty of Medicine, Department of Biotechnology), University J.J. Strossmayer in Osijek in collaboration with University of Dubrovnik and IRB), as principal teachers and collaborators. DMM researchers organize and actively participate in various bachelor's, master's and doctoral courses.

AWARDS

Nela Pivac was awarded the "Ante Šercer" scientific award of the Academy of the Medical Sciences of the Republic of Croatia for the best scientific article published in 2011 from

Croatian authors (Pivac N, Nikolac M, Nedić G, Mustapić M, Borovečki F, Hajnšek S, Presečki P, Pavlović M, Mimica N, Muck-Šeler D (2011) Brain derived neurotrophic factor Val66Met polymorphism and psychotic symptoms in Alzheimer's disease. Progr Neuro-Psychopharmacol Biol Psychiatry, 35: 356-362).

Nela Pivac was appointed an honorary fellow of the Czech Neuropsychopharmacological Society.

Martina Malnar received the L'Oréal-UNESCO "For Women in Science 2012" National Fellowship.

Stjepko Čermak received a Swiss Government scholarship for training at the ETH-Zürich within the project "Imaging of the cannabinoid 2 receptor in brain and spinal cord of mouse models of neurodegenerative and neuroinflammatory diseases by positron emission tomography (PET)".

Ana Šarić and Tanja Matijević obtaned a fellowship financed by Franch embassy in Croatia and IRB for 1 month training in France.

Sonja Levanat received a Terry Fox Run donation, awarded by Embassy of Canada, Croatian League against Cancer, Zagreb holding, Regent Esplanade hotel and Media Val Agency.

Petar Ozretić received a poster award from the European Association for Cancer Research (EACR) at the 2nd Meeting of the Croatian Association for Cancer Research.

Arijana Zorić, Anđela Horvat, Neda Slade, Ivan Sabol and Magdalena Grce received the Annual Ruđer Bošković Institute Director's Prize for excellence in scientific research.

Maja Mustapić received a National Science Foundation scholarship for one-year training at the University of California, San Diego, Institute for Genomic Medicine.

PROJECTS

Programs supported by the Ministry of Sciences, Education and Sports

1. Integrative genomics and proteomics in cancer research. Krešimir Pavelić
2. Pharmacogenomics, proteomics and psychophysiology of neuropsychiatric disorders. Dorotea Muck-Šeler

Projects supported by the Ministry of Sciences, Education and Sports

1. Cytochrome P450 monooxygenase and tumor appearance in ageing and oxidative stress, Tatjana Marotti
2. Gene therapy of tumors by modulating the molecules of the immune system, Jasminka Pavelić
3. The role of nm23 genes in oral squamos cell carcinoma, Maja Herak Bosnar
4. The role of p53/p73 network in soft tissue sarcoma, Neda Slade
5. The mechanism of cholesterol action in the pathogenesis of Alzheimer's disease, Silva Katušić Hećimović
6. Stress, GABA-A receptors and mechanisms of action of neurophychoactive drugs, Dubravka Švob Štrac
7. The role of different cell death responses to DNA-damage treatment, Marijeta Kralj
8. S-Adenosylhomocysteine hydrolase (AHCY) deficiency: Molecular mechanims of a new human disease, Oliver Vugrek
9. Role of membrane peptidases on tumor and normal cells, Jelka Gabrilovac
10. Signal transduction in tumors:Hh-Gli interactions and therapeutic potential, Sonja Levanat
11. Pharmacogenomics and proteomics of serotonergic and catecholaminergic system, Dorotea Mück-Šeler
12. Molecular basis and treatment of psychiatric and stress related disorders, Nela Pivac
13. Lipids, free radicals and their second messengers in integrative oncology, Neven Žarković
14. Molecular genetics and pharmacogenetics of gastrointestinal tumors, Sanja Kapitanović
15. Proteomic prostate tumor biomarker analysis, Mario Cindrić
16. Obtaining the structures like Langherhans islets from mouse stem cells, Mirko Hadžija
17. Aberrant DNA methylation in HPV associated lesions, Magdalena Grce

18. Epigenetic and immunomodulatory changes in malignant head and neck tumours, Koraljka Gall Trošelj

Additional projects at the DMM:

1. New therapeutic modalities in treatment of malignant diseases, Marko Radačić
2. Genetic basis in development of pituitary tumors, Živko Gnjidić
3. Pharmacogenetics in pediatric oncology, Jasenka Stepan Giljević
4. Eye immunology, Iva Dekaris
5. Molecular basis of aseptic instability of hip total endoprotesis, Robert Kolundžić

Research development and international projects

1. Alzheimer disease – the role of cholesterol on processing and localization of APP protein family (Silva Katušić Hećimović, bilateral project with Germany, DAAD)
2. The development of new approaches for molecular and serological diagnostic of human papillomavirus (HPV) infection (Magdalena Grce bilateral project with France)
3. Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain (Dorotea Muck-Šeler, Nela Pivac, COST Project, Action CM1103)
4. Detection and tracking of biological markers for early therapeutic intervention in sporadic Alzheimer's disease (collaborators: Nela Pivac, Dorotea Mück-Šeler, Maja Mustapić, Matea Nikolac, Gordana Nedić, Dubravka Švob Štrac, Maja Jazvinščak Jembrek, Croatian Science Foundation).
5. Molecular profiling and proteomics of urothelial carcinoma (collaborator Neda Slade, Croatian Science Foundation "Partnership in Research").
6. Genetic testing of monogenetic diseases: cystic fibrosis, non-syndromic deafness, Rett syndrome, (Jasminka Pavelić, Clinical Hospital Center Split, Children's Hospital Zagreb).
7. SAHH deficiency: Epigenetic characterization of a novel human methylation disorder (Oliver Vugrek, bilateral project with Germany, DAAD; Institute for Human Genetics, Mainz)

SELECTED INVITED LECTURES

1. Pivac N. Biomarkers as new tools to improve the diagnosis and treatment of PTSD. NATO Science for peace programme: NATO ASI - Invisible Wounds, New Tools to Enhance PTSD Diagnosis and Treatment, Ankara, Turkey, June 19-23, 2012.
2. CM1103 Action: "Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain", 1st WG4 Scientific Meeting Monoamines and Drugs: New Insights into the Brain Disorders, 26-27 April 2012, Zagreb, Croatia:
   Muck-Šeler D: Proteins of the serotonergic system and drugs
   Pivac N: Monoaminergic background and pharmacotherapy of psychotic subtype of PTSD
   Mustapić M: Noradrenergic system in Alzheimer's disease
   Nedić G: Dopaminergic system in alcoholism
   Nikolac M: Monoaminergic background of ADHD
   Švob Štrac D: Recombinant receptors-model for neuropharmacological studies
   Jazvinščak Jembrek M: P19 neurons as a model to study protective effects of monoamines against oxidative injury
   Vlainić J: The effects of fluoxetine under the conditions of stress
3. Muck-Šeler D. New development in Alzheimer's Disease. COST CM 1103 Action, Madrid, Spain, November 24, 2012.
4. Hećimović Katušić S. The molecular links between lysosomal storage diseases and Alzheimer's disease, Workshop: New Developments of Lysosomal storage disease diagnostics & therapeutics: LSD Protein – aggregation & interactions, University of Konstanz, Germany, March 15, 2012.

5. Hećimović Katušić S. The link between NP-C and Alzheimer's disease, Actelion's joint international advisory board on Niemann-Pick Type C, Zurich, Switzerland, May 10, 2012.
6. Levanat S: The Hedgehog-Gli signaling in tumors and implications for therapy, FEBS 3+ meeting, Opatija, Croatia, June 13-16, 2012.
7. Levanat S: Hedgehog signaling in cancer and therapeutic potential, 1st Scientific meeting of the Serbian Association for Cancer Research, Belgrade, Serbia, November 29-30,2012
8. Grce M. Cervical cancer prevention programs. Meeting regarding the beginning of development of program for cervical cancer prevention in Bosnia & Herzegovina, Parliamentary Assembly of Bosnia & Herzegovina, Sarajevo, Bosna & Hercegovina, July 25, 2012.
9. Grce M. Organised screening programs in the era of HPV vaccination. 37th European Congress of Cytology, Dubrovnik-Cavtat, Croatia, September 30 – October 3, 2012.
10. Grce M. Oncogenic HPV and cervical cancer. 3rd International Congress of Kosovo and Albanian Oncologist, Prishtina, Kosovo, November 2 – 3, 2012.
11. Gall Trošelj K. Curcumin as a modifier of histone methylating enzymes expression. Invited by Korean Society of Food Science and Technology. Seoul, Koreja, April 26, 2012.
12. Vugrek O: New insights in intracellular dynamics of S-Adenosylhomocysteine hydrolase, a key enzyme for methionine metabolism; FEBS 3+ meeting, Opatija, Croatia, June 13-16, 2012.
13. Vugrek O: Ten years of S-Adenosylhomocysteine hydrolase deficiency: a unique model system for methylation research in human; July 11th, 2012, Institute for Human Genetics, Mainz, Germany.

SELECTED ORGANIZED CONFERENCES

1. Workshop on miRNAs and Virus-Associated Cancers, Dubrovnik, Croatia, May 26-28, 2012. (Grce M)
2. Vaccination and fight against infectious diseases and cancer. What we do for ourselves? What society can do for us? Public tribune, Tribune of the City of Zagreb, Zagreb, Croatia, January 24, 2012. (Grce M)
3. 1st COST CM 1103 Action: 1st WG 4 scientific meeting: Monoamines in the etiology and treatment in neurodegenerative and psychiatric disorders: basic and clinical investigations, Zagreb, Croatia, April 26-27, 2012 (Muck-Šeler D and Pivac N)
4. 6th Croatian Congress on Alzheimer's disease with international participation, Primošten, Croatia, October 10-13, 2012 (Pivac N and Muck-Šeler D)
5. Federation of European Biochemical Society Meeting (FEBS 3+): From molecules to life and back. 13-16.6. 2012 Opatija, Croatia (Balog T and Levanat S)
6. Second Meeting of the Croatian Association for Cancer Research with international participation, HDIR-2 ''From Bench to Clinic'', Zagreb, Croatia,November 8-9, 2012. (Levanat S, Herak Bosnar M, Slade N, Car D, Levačić Cvok M, Musani V, Ozreić P, Sabol M)

SELECTED PUBLICATIONS

1. Muck-Šeler D, Pivac N, Dikšić M. Acute treatment with fluvoxamine elevates rat brain serotonin synthesis in some terminal regions: An autoradiographic study. *Nucl Med Biol* **39** (2012) 1053.
2. Podobnik J, Foller Podobnik I, Grgić N, Marčinko D, Pivac N. The effect of add-on treatment with quetiapine on measures of depression, aggression, irritability and suicidal tendencies in children and adolescents. *Psychopharmacology* **220** (2012) 639.
3. Šagud M, Nikolac M, Mihaljević-Peleš A, Nedić G, Vuksan Ćusa B, Mustapić M, Jakovljević M, Muck-Šeler D, Pivac N. The lack of effect of ziprasidone on platelet serotonin concentration in schizophrenic patients. Letter to the editors. *Psychopharmacology* **219** (2012) 1179.
4. Jelaković B, Karanović S, Vuković-Lela I, Miller F, Edwards K, Nikolić J, Tomić K, Slade

N, Brdar B, Turesky R, Stipančić Ž, Dittrich D, Grollman A, Dickman K. Aristolactam-DNA adducts are a biomarker of environmental exposure to aristolochic acid. *Kidney Int* **82** (2012) 559.
5. Horvat T, Mužinić A, Barišić D, Herak Bosnar M, Zoldoš V. Epigenetic modulation of the HeLa cell membrane N-glycome. *Biochim Biophys Acta - Gen Subj* **1829** (2012) 1412.
6. Knežević J, Pavlinić D, Rose II WA, Leifer CA, Bendelj K, Gabrilovac J, Parcin M, Lauc G, Kubarenko AV, Petričević B, Vrbanec D, Bulat-Kardum L, Bekeredjian-Ding I, Pavelić J, Dembić Z, Weber AN. Heterozygous carriage of a dysfunctional TLR9 allele affects CPG-oligonucleotide responses in B cells. *J Biol Chem* **287** (2012) 24544.
7. Malnar M, Košiček M, Lisica A, Posavec M, Krolo A, Njavro J, Omerbašić D, Tahirović S, Hećimović S. Cholesterol-depletion corrects APP and BACE1 misstrafficking in NPC1-deficient cells. *Biochim Biophys Acta - Mol Basis Dis* **1822** (2012) 1270.
8. Ester K, Supek F, Majsec K, Marjanović M, Lembo D, Donalisio M, Smuc T, Jarak I, Karminski-Zamola G, Kralj M. Putative mechanisms of antitumor activity of cyano-substituted heteroaryles in HeLa cells. *Invest New Drugs* **30** (2012) 450.
9. Aleksić M, Bertoša B, Nhili R, Uzelac L, Jarak I, Depauw S, David-Cordonnier M-H, Kralj M, Tomić S, Karminski-Zamola G. Novel Substituted Benzothiophene- Thienothiophene-carboxanilides, quinolones: Synthesis, Photochemical Synthesis, DNA–binding Properties, Antitumor evaluation, QSAR analysis. *J Med Chem* **55** (2012) 5044.
10. Perković I, Butula I, Kralj M, Martin-Kleiner I, Balzarini J, Hadjipavlou-Litina D, Katsori A-M, Zorc B. Novel NSAID 1-acyl-4-cycloalkyl/arylsemicarbazides and 1-acyl-5-benzyloxy/hydroxy carbamoylcarbazides as potential anticancer agents and antioxidants. *Eur J Med Chem* **51** (2012) 227.
11. Kašnar-Šamprec J, Ratkaj I, Mišković K, Pavlak M, Baus-Lončar M, Kraljević Pavelić S, Glavaš-Obrovac LJ, Žinić B. In vivo toxicity study of N-1-sulfonylcytosine derivatives and their mechanisms of action in cervical carcinoma cell line. *Invest New Drugs* **30** (2012) 981.
12. Sabol I, Matovina M, Si-Mohamed A, Grce M. Characterization and whole genome analysis of human papillomavirus type 16 e1-1374^63nt variants. *PLoS One* **7I7** (2012) e41045.
13. Marković Z, Milenković D, Đorović J, Dimitrić Marković J, Stepanić V, Lučić B, Amić D. PM6 and DFT study of free radical scavenging activity of morin. *Food Chem* **134** (2012) 1754.
14. Marković Z, Milenković D, Đorović J, Dimitrić Marković J, Stepanić V, Lučić B, Amić D. Free radical scavenging activity of morin 2'-O− phenoxide anion. *Food Chem* **135** (2012) 2070.
15. Racané L, Kraljević Pavelić S, Ratkaj I, Stepanić V, Pavelić K, Tralić-Kulenovića V, Karminski-Zamola G. Synthesis and antiproliferative evaluation of some new amidino-substituted bis-benzothiazolyl-pyridines and pyrazine. *Eur J Med Chem* **55** (2012) 108.
16. Stepanić V, Žiher D, Gabelica-Marković V, Jelić D, Nunhuck S, Valko K, Koštrun S. Physicochemical profile of macrolides and their comparison with small molecules. *Eur J Med Chem* **47** (2012) 108.
17. Leović D, Sabol M, Ozretić P, Musani V, Car D, Marjanović K, Zubčić V, Sabol I, Sikora M, Grce M, Glavaš-Obrovac L, Levanat S. Hh-Gli signaling pathway activity in oral and oropharyngeal squamous cell carcinoma. *Head Neck - J Sci Spec Head Neck* **34** (2012) 104.

Review Articles

1. Grce M, Sabol I, Milutin Gašperov N. Burden and prevention of HPV related diseases: Situation in Croatia. *Period Biol* **114** (2012) 175.
2. Grce M, Sabol I, Milutin Gašperov N. The transforming properties of human papillomavirus oncoproteins. *Period Biol* **114 (**2012) 479.
3. Gomaz A, Pavelić J, Matijević Glavan T. The polymorphisms in Toll-like receptor genes and cancer risk. *Period Biol* **114 (**2012) 461.
4. Deželjin M, Herak Bosnar M. Metastasis – recent scientific insights and challenging

new therapeutic approaches. *Period Biol* **114** (2012) 453.
5. Ozretić P, Bisio A, Inga A, Levanat S. The growing relevance of cap-independent translation initiation in cancer-related genes. *Period Biol* **114** (2012) 471.
6. Sirotković M, Kulić A, Bracić L, Čačev T. Protumor effects of proinflammatory mediators in breast cancer. *Period Biol* **114 (**2012) 489.

CHAPTERS IN BOOKS

1. Pivac N, Nedić G, Nikolac M, Fistonic M, Kovacevic M, Mustapić M, Gveric Korkut I, Grubisic-Ilic M, Kozaric-Kovacic D, Muck-Seler D (2012) Neurobiological basis of pain syndrome in war veterans with PTSD: preliminary findings. In: Pain syndromes – From Recruitment to returning troups: Wounds of War IV. Wiederhold, Brenda K. (ed). Amsterdam: IOS Press, pp 94-122
2. Švob Štrac D, Vlainić J, Jazvinšćak Jembrek M, Muck-Šeler D, Pivac N. The Effects of Benzodiazepines during Prolonged Administration and Under the Conditions of Stress. In: Benzodiazepine: Abuse and Therapeutic Uses, Pharmacology and Health Effects. Soto AL, Reyes CF (eds.). New York, USA: Nova Science Publishers, Inc. pp. 1-54.
3. Gall Trošelj, K, Novak Kujundžić R, Grbeša I (2012). The importance of aberrant DNA methylation in Cancer, DNA Methylation - From Genomics to Technology. Tatarinova T (ed.), ISBN: 978-953-51-0320-2, InTech, DOI: 10.5772/35820. Available from: http://www.intechopen.com/books/dna-methylation-from-genomics-to-technology/the-importance-of-aberrant-dna-methylation-in-cancer

Division of Marine and Environmental Research

http://www.irb.hr/en/zimo

DIVISIONAL ORGANIZATION

Head: Tarzan Legović

The Division for Marine and Environmental Research (DMER) consists of the following laboratories:

- Laboratory for Satellite Oceanography, Milivoj Kuzmić
- Laboratory for Informatics and Environmental Modelling, Tarzan Legović
- Laboratory for Physical Chemistry of Aquatic Systems, Irena Ciglenečki Jušić
- Laboratory for Physical Chemistry of Traces, Milivoj Lovrić
- Laboratory for Inorganic Environmental Geochemistry, Goran Kniewald
- Laboratory for Analytical Chemistry and Biogeochemistry of Organic Compounds, Marijan Ahel
- Laboratory for Bioelectrochemistry and Surface Imaging, Vesna Svetličić
- Laboratory for Radioecology, Delko Barišić
- Laboratory for Biological Effects of Metals, Marijana Erk
- Laboratory for Molecular Ecotoxicology, Tvrtko Smital
- Laboratory for Aquaculture and Pathology of Aquatic Organisms, Emin Teskeredžić

OVERVIEW OF THE DIVISION

The mission of the Division is to expand and deepen our leadership in fundamental and applied studies of environmental systems, processes and states. Our research is oriented toward the optimization of environmental management for the benefit of our country and the world.

During 2012, division scientists worked on more than 50 research projects contracted by the Ministry of Science, Education and Sport and outside clients. These projects spanned a wide range of topics in marine and environmental science, ranging from satellite oceanography down to nanotechnology. Research results were published in 70 scientific papers in journals indexed by Current Contents and 10 papers in other scientific journals, 3 book chapters, a number of conference proceedings and technical reports. In addition, 12 invited lectures were held, 7 conferences were organized, 4 graduate schools were coordinated and 3 Ph.D and 2 B.Sc. theses were defended under the mentorship of division scientists. Finally, 23 undergraduate and 76 post-graduate courses were given at universities in Croatia and abroad.

TOP ACHIEVEMENTS

Wave contribution to currents near the surface of the Adriatic Sea

Implementation of the Regional Ocean Modelling System (ROMS), two-way coupled to the Wind Wave Model II (WWM II), was used as the computational platform for numerical experiments designed to evaluate the wave contribution to dynamics in the near surface region. Recent concepts in the physics of spectral wave modelling were applied to close the momentum balance in the surface boundary layer. To force the ROMS and WWM II models and to assess their modelling skill we used observations and model results made during 2002 and 2003 in the Adriatic Sea. When all effects were included in the simulation, comparison with top-bin Acoustic Doppler Current Profilers (ADCP) measurements showed improvements. Our results also point to the importance of computing the Stokes drift from the full wave spectra instead of using a simplified truncation formula (Dutour Sikirić et al., 2012).

Determination of sulfated polysaccharides in seawater

The method of adsorptive transfer chronopotentiometric stripping was applied for the first time to the determination of sulfated polysaccharides in natural seawater. The method also has applications to other media where direct determination of polysaccharides is not possible (Strmečki and Plavšić, 2012)

Determination of surfactants in atmospheric aerosol

A novel analytical approach (out-of-phase AC voltammetry) for the direct qualitative and quantitative characterisation of surfactants in atmospheric aerosol water extracts, rain and cloud water was proposed (Frka et al., 2012).

Voltammetric investigation of iron(III) complexes with siderophore chrysobactin in aqueous solution

Voltammetric investigations of iron(III) complexes with siderophore chrysobactin were performed in order to clarify complex stoichiometry, as well as reduction mechanism. These studies are of biological importance since they provide an insight into the possible reduction mechanism found in bacterial cells that use chrysobactin to acquire iron (Vukosav et al., 2012).

Revision of iron(III)-citrate speciation in aqueous solution: Voltammetric and spectrophotometric studies.

Iron(III) complexes with citric acid as a ligand have been investigated, due to their importance for iron speciation in different (eco)systems (sea, freshwater systems, atmosphere, living world). By using voltammetric and UV-Vis spectrophotometric techniques different iron(III)-citrate species were characterized (their stoichiometry and stability constants were determined), (Vukosav et al., 2012a).

Theory of square-wave voltammetry of two electron reduction with an intermediate that is stabilized by complexation

The intermediate of a two-step, reversible electrode reaction is stabilized by complexation if the separation of two peaks of the split net response increases with increasing ligand concentration. The relationship between the potential of the second peak and the logarithm of ligand concentration tends to the asymptote with a slope that is proportional to the maximum number of ligands bound to the intermediate. If only the intermediate forms complexes, the relationships between potentials of the first and second peaks and

the logarithm of ligand concentration are symmetrical. The potentials of the first peak are a convex function of the logarithm of ligand concentration if the reactant also forms complexes with the ligand. The number of electrons can be estimated from the half-peak widths (Komorsky-Lovrić and Lovrić, 2012).

The distribution of iodine in the Croatian marine lake, Mir – The missing iodate

The marine chemistry of iodine has been studied in the marine lake, Mir, regarded as a natural reactor situated in the karstificated carbonate rocks of the Croatian Adriatic coast. Lake Mir was found to be meso-trophic, with dynamic nutrient cycling of a magnitude usually associated with the temperate zone but within a Mediterranean clime. The chemistry of iodine in Lake Mir is consequently dominated by changes in iodide and organic-I concentrations, with the latter being at higher concentrations than those found in seawater (Žic et al., 2012)

Circumstantial evidence in support of org-I as a component of the marine aerosol arising from a study of marine foams

A study of foams formed on the marine Lake Mir, Croatia, and elsewhere on the same coast demonstrates, that they are fractionated (enrichened) in org-I by up to 630 times relative to the water from which they form. Since foam production is ubiquitous over the oceans it seems likely that this process local to coastal environments is much more common than might first appear to be the case. This work provides circumstantial evidence that the bubble-bursting mechanism current since the 1960s may well provide the iodine which appears to be missing in many modelling calculations based upon an atmospheric system dependent upon sorption of the species IO upon the marine aerosol (Truesdale et al., 2012).

Reaction kinetics and mechanical models of liposome adhesion at charged interface

Reaction kinetics and mechanical models were applied to an analysis of amperometric signals to explore the dynamics of liposome adhesion at a mercury interface. The reaction kinetics model identifies the temporal evolution of three distinct states, while a mechanical model provides a physical interpretation of these states and describes water release through transient pores formed in the cap membrane (Ivošević DeNardis et al., 2012).

Surface modified liposomes by mannosylated conjugates anchored via the adamantyl moiety in the lipid bilayer

The study of encapsulated mannosylated 1-aminoadamantane and mannosylated adamantyltripeptidesin liposomes has revealed that the encapsulation of the examined compounds, increases liposome size and changes their surface morphology. The enlargement of liposomes was ascribed to the specific binding of the added ConA moiety to the mannose present on the surface of the prepared liposomes (Štimac et al., 2012).

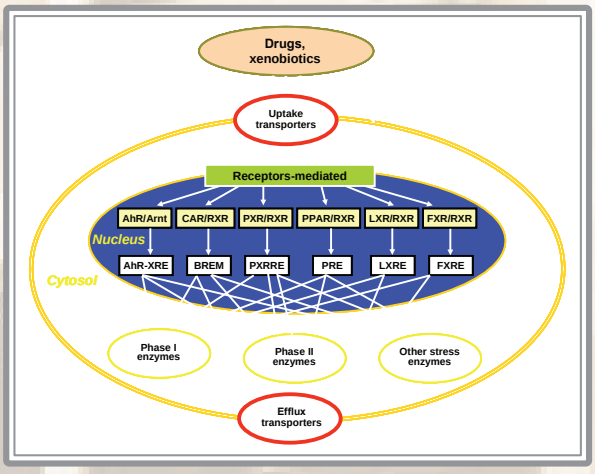


Fig. 1. Schematic presentation of the role of specific transmembrane proteins in cellular detoxification and stress responses in aquatic organisms.

Unusual pathway of zeolite ZSM-5 crystallization in a heterogeneous system: phenomenology and starting considerations

This article defined the crystallization process of zeolite ZSM-5 from a diluted heterogeneous system, showing that crystallization takes place through a chain of processes from formation of “primary” amorphous aluminosilicate precursors through formation of “secondary” and tertiary” amorphous aluminosilicate precursors and finally formation of nuclei and their growth (Ren et al., 2012).

The evolution of atrazine-degrading capabilities in the environment

A comprehensive overview of the enzymes involved in atrazine mineralization and their evolutionary histories is presented. The genetic composition of microbial populations involved in atrazine degradation and the biotechnologies that have been developed, based on these systems, for the bioremediation of atrazine contamination in the environment has been discussed (Udiković-Kolić et al., 2012).

Chronic exposure of feral fish to elevated Pb concentrations in river water

Lead concentrations were determined by HR ICP-MS in the gill and hepatic soluble fractions of European chub (Squalius cephalus) caught in the Sutla River (Croatia–Slovenia border). The fact that Pb increases in gilsl and hepatic soluble fractions of the European chub was not caused by biotic factors and was spatially restricted to one site with increased dissolved Pb concentration in the river water. This result points to the applicability of this parameter as an early indicator of Pb exposure in monitoring of natural waters (Dragun et al., 2012).

Gastrointestinal metal variability of indigenous European chub from the Sava River

This comprehensive field survey presents, for the first time, the site-specific variability of trace metal concentrations in the gut content, gastrointestinal tissue and two gastrointestinal sub-cellular fractions, operationally defined as metal-sensitive fraction and metal detoxified fraction. Site-specific differences point to the age-related increase of gastrointestinal Cu, Mn and Cd towards downstream sites, while a significant correlation between metal concentrations in the gut content and fish age exists only for Mn. The observed differences in metal abundance between gut content and gastrointestinal tissue points to selective metal absorption in fish intestines (Filipović Marijić and Raspor, 2012).

Targeting mussel tissue for cellular energy allocation (CEA) as a biomarker in Mytilus galloprovincialis

Three selected mussel tissues (digestive gland, mantle, and gills) were studied to determine which was the most suitable for the potential use of the cellular energy allocation (CEA) methodology in indigenous mussels Mytilus galloprovincialis. The CEA value was calculated as the ratio between available energy (Ea) and energy consumption (Ec). Greater Ec in mussels from an estuarine site than from a coastal site was detected only in the digestive gland tissue, and can probably be attributed to the energetically costly maintenance of osmotic balance. Using digestive gland tissue in CEA analysis demonstrated a clear difference between coastal and estuarine sampling sites, providing a measure of the natural stress posed by variations in salinity (Erk et al., 2012).

Molecular characterisation of Anisakidae larvae isolated from fish in the Adriatic Sea

The occurrence of Anisakis typica in Thunus thynnus is the first case of this species found in the Adriatic Sea and extends its geographical distribution previously limited to other regions and host species of the Mediterranean Sea. Co-infection of Hysterothylacium aduncum with Anisakis type I larvae found in mackerels from a fish market is a matter of human health concern, since these species have been identified as agents of human anisakiasis and allergy (Vardić et al., 2012).

A novel type of colony formation in marine planktonic diatoms revealed by atomic force microscopy

A novel strategy for colony formation in marine planktonic diatoms is revealed by atomic force microscopy (AFM). An optically transparent organic matrix, enclosing Bacteriastrum jadranum cells, was visualized at molecular resolution as a highly organised and delicately structured fibrillar network (Bosak et al., 2012).

Effects of maximum sustainable yield on competitive and mutualistic communities

A maximum sustainable yield (MSY) for fishery has been advocated by the Johannesburg Plan of Implementation, 2002 and the EU green Paper on fishery reform, 2009. It has been found that MSY most likely will lead to the loss of species in both competitive (Geček and Legović, 2012) and mutualistic communities (Legović and Geček, 2012) and this is contrary to the precautionary principle and violates the Convention of Biological Diversity, 1992.

Nanomechanical characterization of eye lens cells stiffness: A pilot study

Mechanical properties of individual cortical and nuclear lens cells are probed using atomic force spectroscopy under basal conditions and after addition of cytoskeletal drugs. The uncommon maintenance of shape and elastic properties after cell isolation together with the null effect of actin filament and microtubule targeting drugs suggest that the mechanical stability of fiber cells is provided by cellular elements other than the usual cytoskeletal proteins (Hozić et al., 2012).

Risk assessment of the intake of pesticides in Croatian diet

For the first time, a comprehensive study of the exposure of the Croatian population to pesticide residues through fruit and vegetable consumption was assessed based on the 2007-2009 surveillance data. The short-term exposure assessment revealed that for 12 food samples analyzed the acute reference dose (ARfD) might have been exceeded if the food sample was consumed in high amounts, however, the long-term exposure of consumers did not raise health concerns (Knežević et al., 2012).

Comparing illicit drug use in 19 European cities through sewage analysis

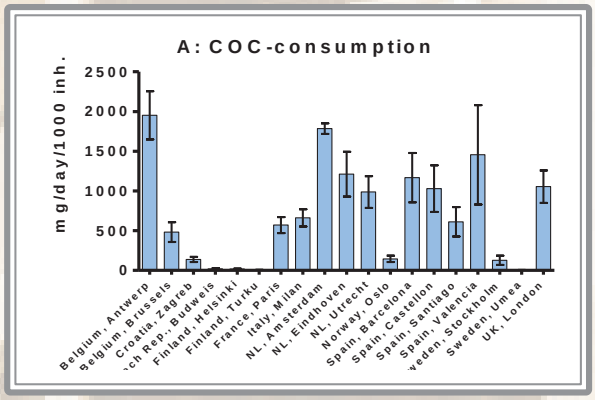


Fig. 2. Comparison of cocaine consumption in 19 European cities through sewage analysis

The analysis of sewage for urinary biomarkers is a promising approach for estimating the use of illicit drugs by the general population. For the first time, this approach was simultaneously applied in 19 European

cities, making it possible to directly compare illicit drug loads in Europe. This study shows that a standardized analysis for illicit drug urinary biomarkers in sewage can be applied to estimate and compare the use of these substances at local and international scales. The approach has the potential to deliver important information on drug markets (Thomas et al., 2012).

EDUCATION

Division members teach 23 undergraduate and 76 post-graduate courses.at all universities in Croatia and several universities abroad. In addition, they help coordinate four Ph.D. schools: ***Environmental Management*** and ***Oceanology*** with the University of Zagreb, ***Biophysics*** with the University of Split, and ***Environmental Protection and Nature Conservation*** with the University J.J. Strossmayer in Osijek.

AWARDS

1. Galja Pletikapić: L'oreal- Unesco "For Woman in Science" National fellowship.
2. Damir Kapetanović: The Macedonian Ecological Society, for the best poster.
3. Galja Pletikapić: "Jean Giaja" young scientist prize for the best poster.
4. Galja Pletikapić: Croatian Science Foundation Doctoral Fellowship.
5. Ivan Senta, Senka Terzić, Marijan Ahel, Slađana Strmečki, Vesna Svetličić, Tea Mišić Radić, and Amela Hozić: RBI Award, for outstanding publication

PROJECTS

Programs supported by the Ministry of Science, Education and Sports

1. Biogeochemical Processes and Environmental Risk, Marijan Ahel

Projects supported by the Ministry of Science, Education and Sport

1. Organic compounds as molecular biomarkers of antropogenic impact, Marijan Ahel
2. Metal-induced cellular changes in aquatic organisms, Biserka Raspor
3. Radionuclides and trace elements in environmental systems. Delko Barišić
4. Nature of organic matter, interaction with traces and surfaces in environment, Irena Ciglenečki-Jušić
5. Mathematical modeling of circulation and satellite sensing of boundary processes, Milivoj Kuzmić
6. Pathology of aquatic organisms in relation to pollution and aquaculture, Emin Teskeredžić
7. Electroactive films for ecologically acceptable energy conversion and storage, Višnja Horvat-Radošević
8. Electroanalytical research on microcrystals and traces of dissolved substances, Milivoj Lovrić
9. Interactions of trace metal species in an aquatic environment, Ivanka Pižeta
10. Ecotoxicological significance of ABC transport proteins in aquatic organisms, Tvrtko Smital
11. Surface forces on atomic scale applied in marine science and nanotechnology. Program leader: Vesna Svetličić
12. Biogeochemistry of metals in sedimentary systems and soils in Croatia, Goran Kniewald
13. Ecological modelling for sustainable management of resources, Tarzan Legović
14. Information systems for environmental quality and risk assessment, Jadranka Pečar-Ilić
15. Networked Economy, Jadranka Pečar-Ilić
16. Systematic study of the Adriatic Sea as a basis for sustainable development of the Republic Croatia, Croatian National Monitoring Programme of the Adriatic Sea.

Selected research, developmental and international projects

1. Innovative biodiagnosis meets chemical structure elucidation – novel tools in effect directed analysis to support the identification

and monitoring of emerging toxicants on a european scale (EDA-EMERGE). FP7 Marie Curie ITN project (2011-2015), Project no. 290100; Project coordinator Werner Brack; PI for IRB Marijan Ahel.

2. Development and evaluation of innovative tools to estimate the ecotoxicological impact of low dose pesticide application in agriculture on soil functional microbial biodiversity (acronym ECOFUN-MICRODIV); co-funded by the European Community's Programme for International Cooperation under the 7th Framework Programme for Research and Technological Development (2007-2013); number of the project SEE-ERA-NET 216; PI for IRB Ines Petrić.
3. Bilateral Croatian-(FYR)Macedonian project: "The assessment of metal availability and effects on feral fish in the rivers under the impact of mining activites" (Croatian partner: RBI, DMER, Laboratory for biological effects of metals, project leader: Zrinka Dragun; (FYR)Macedonian partner: Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University in Skopje, project leader: Maja Jordanova).
4. „Nanoparticles in aqueous environment: electrochemical, nanogravimetric, STM and AFM studies" ,Irena Ciglenečki-Jušić, UKF.
5. Croatian-Macedonian bilateral project, ''BActerial and ParasiTical communities of chub as Indicators of the Status of environment exposed to Mining activities – BAPTISM'', leader: Damir Kapetanović, source of finance: Croatian Ministry of Science, Education and Sport, number of project: 910-08/11-01/00257.
6. Trace ecotoxic metals determination in water, sediments and biota in the aquatorium of Nature Park "Telašćica, Marina Mlakar, PU Telašćica.
7. Carrying capacity for tourists in the Narional Park Krka, NP Krka, Legović Tarzan
8. Natural concentrations of metals in coastal water according to Water Frame Directive, Marina Mlakar, Croatian Waters.
9. Calibrations of paleoenvironmental records in (sub)recent tufa, Neven Cukrov, bilateral with Slovenia.
10. Determination of ecotoxic metals in water environment of Rijeka harbor using passive samplers, Neven Cukrov, Port of Rijeka Authority.
11. Influence of the water mass circulation on spatial and temporal distribution of ecotoxicants in Malo jezero and Veliko jezero lakes of Mljet National park, Vlado Cuculić, NP Mljet.
12. Trace metals analysis in subterranean waters of Petruševec water well's, Neven Cukrov, City of Zagreb.
13. Study of electrochemical methods for the detection of trace metals in seawater, French defence agency (DGA), Leader: C. Garnier; CRO Collaborators: D. Omanović, I. Pižeta and M. Lovrić.
14. An impact of antifouling paints as a source of contamination by ecotoxic metals in the coastal marine environment, COGITO (FRA-CRO) project, Leaders: C. Garnier (FRA), D. Omanović (CRO).
15. Gold microwire: a new tool for trace metal speciation in natural waters, UK Royal Society of Chemistry, Leaders: P. Salaun (UK), D. Omanović (CRO).
16. Comparison of paleoenvironmental data from tufa precipitate in Croatia, Slovenia and Spain. N. Cukrov, Spanish Ministry of Science and Innovation.
17. Establishing and developing of an ecotoxicology platform in Serbia and Croatia: a focus on zebrafish (Danio rerio), Tvrtko Smital – Swiss National Science Fondation (SNSF), SCOPES 2009-2013: Joint Research Project;
18. COST Action TD 1002 (2010-2014), European network on applications of atomic force microscopy to nanomedicine and life science, V. Svetličić (coordinator of WG 4: Environmental Nanotoxicology and Nanoparticles and member of Core Management)

SELECTED INVITED LECTURES

1. Plavšić Marta, Strmečki Kos Slađana, Adsorptive Transfer Chronopotentiometric Strip-

ping of Sulfated Polysaccharides Applied to Seawater Analysis. 45th Heyrovsky Discussion; Electrochemistry of Biopolymersand Bioactive Compounds. Brno, Czech Republic, August 13-17, 2012.

2. Irena Ciglenečki, Rogoznica Lake (Croatia), a unique anoxic seawater system on the Adriatic coast", Ben-Gurion, University of the Negev, Department of Geological and Environmental Sciences, Izrael, October 2012.
3. Valić Damir, Farmed Sea bass (*Dicentrarchus labrax*) in Eastern Adriatic: Seasonal and regional differences in parasitofauna, «AQUA 2012: Global Aquaculture – Securing Our Future», Czech Republic, September 1-5, 2012.
4. Smital T: Uptake and efflux transport proteins as integral elements of the cellular detoxification and environmental stress response in aquatic organisms. 28th ESCPB Congress (European Society for Comparative Physiology and Biochemistry), Bilbao, Spain, Sep 2-5, 2012.
5. Vesna Svetličić, Galja Pletikapić, Ivana Vinković Vrček, Vera Žutić, Marine biopolymers and nanoparticles interaction, Regional Biophysical Conference, Kladovo, Serbia, September 3-9, 2012
6. Galja Pletikapić, Tea Mišić Radić, Alex Berquand, Unige Murvai, Miklos Kellermayer, Ivana Vinković Vrček, Vera Žutić, Vesna Svetličić, Marine diatom cells and extracellular polymers: nanostructure, nanomechanics and interactions with nanoparticles, From Solid State To BioPhysics VI From Physics To Life Sciences, Cavtat, Croatia, June 9-16, 2012
7. Vesna Svetličić, Persistence of engineered nanoparticles in marine environment, Nanobiotechnology International Workshop, JRC, Ispra, Italy, December 4-6, 2012
8. Vesna Svetličić, The use of Atomic Force Microscopy for the imaging of nanoparticles including pilot experiments with nanosilver garment, COST Action BM0903 Skin Barrier in Atopic Dermatitis (SKINBAD) Zagreb, Croatia, December 13-14, 2012

SELECTED ORGANIZED CONFERENCES

1. The third day of electrochemistry" in memory of Marko Branica, RBI, April 26, 2012. Š. Komorsky Lovrić, V. Cuculić.
2. "ISE Satellite Student Regional Symposium on Electrochemistry", RBI, April 26, 2012. Dijana Jadreško.
3. 2nd International Symposium on "Anchialine Ecosystems", Cavtat, Croatia, October 3-6, 2012. N. Cukrov.
4. Voltammetry and Geotraces, A COST Action ES0801 Workshop, Šibenik, Croatia, October 6-9, 2012. I. Ciglenečki Jušić, D. Omanović, I. Pižeta.
5. Vesna Svetličić (Scientific board) Regional biophysics conference 2012, Kladovo, Serbia.
6. Amela Hozić, Galja Pletikapić, Vesna Svetličić (Organizing Committee) 11th Greta Pifat-Mrzljak International School of Biophysics, 2012, Primošten, Croatia.
7. Nadica Ivošević DeNardis (Organizing Committee) 2nd Adriatic school of nanoscience (ASON-2), From Synthesis to Characterization, 2012, Dubrovnik, Croatia.

SELECTED PUBLICATIONS

1. Thomas KV, Bijlsma L, Castiglioni S, Covaci A, Emke E, Grabic R, Hernández F, Karolak S, Kasprzyk-Hordern B, Lindberg RH, Lopez de Alda M, Meierjohann A, Ort C, Pico Y, Quintana JB, Reid M, Rieckermann J, Terzić S, van Nuijs ALN, de Voogt P. Comparing illicit drug use in 19 European cities through sewage analysis. *Sci Tot Environ* **432** (2012) 432.
2. Dunstan MS, Barkauskaite E, Lafite P, Knežević CE, Brassington A, Ahel M, Hergenrother PJ, Leys D, Ahel I. Structure and mechanism of a canonical poly(ADP-ribose) glycohydrolase *Nature Commun* **3** (2012) 878.
3. Knežević Z, Serdar M, Ahel M. Risk assessment of the intake of pesticides in Croatian diet. *Food Control* **23** (2012) 59.
4. Rožmarić M, Rogić M, Benedik Lj, Štrok M.

Natural radionuclides in bottled drinking waters produced in Croatia and their contribution to radiation dose. *Sci Tot Environ* **437** (2012) 53.
5. Rožmarić M, Rogić M, Benedik Lj, Štrok M, Barišić D, Gojmerac Ivšić A. ^{210}Po and ^{210}Pb activity concentrations in *Mytilus galloprovincialis* from Croatian Adriatic coast with the related dose assessment to the coastal population. *Chemosphere* **87** (2012) 1295.
6. Dragun Z, Krasnići N, Strižak Ž, Raspor B. Lead concentration increase in the hepatic and gill soluble fractions of European chub (*Squalius cephalus*) - an indicator of increased Pb exposure from the river water. *Environ Sci Pollut Res* **19** (2012) 2088.
7. Strmečki S, Plavšić M. Adsorptive transfer chronopotentiometric stripping of sulphated polysaccharides. *Electrochem Comm* **18** (2012) 100.
8. Frka S, Dautović J, Kozarac Z, Ćosović B, Hoffer A, Kiss G. Surface active substances in atmospheric aerosol: an electrochemical approach. *Tellus. Series B, Chem Phys Meteorology* **64** (2012) 1.
9. Dutour Sikirić M, Roland A, Tomažić I, Janeković I. Hindcasting the Adriatic Sea near-surface motions with a coupled wave-current model. *J Geophys Res-Oceans*, **117** (2012) C00J36.
10. Supić N, Kraus R, Kuzmić M, Paschini E, Precali R, Russo A, Vilibić I. Predictability of northern Adriatic winter conditions. *J Marine Systems* **90** (2012) 42.
11. Janeković I, Powell B. Analysis of Imposing Tidal Dynamics to Nested Numerical Models. *Cont Shelf Res* **34** (2012) 30.
12. Vardić Smrzlić I, Valić D, Kapetanović D, Kurtović B, Teskeredžić E. Molecular characterisation of Anisakidae larvae from fish in Adriatic Sea. *Parasitol Res* **111.6** (2012) 2385.
13. Cukrov N, Tepić N, Omanović D, Lojen S, Bura-Nakić E, Vojvodić V, Pižeta I. Qualitative interpretation of physico-chemical and isotopic parameters in the Krka River (Croatia) assessed by multivariate statistical analysis. *Int J Environ Anal Chem* **92** (2012) 1187.
14. Frančišković-Bilinski S, Bhattacharya AK, Bilinski H, Bhattacharya BD, Mitra A, Sarkar SK. Fluvial geomorphology of the Kupa River drainage basin, Croatia: A perspective of its application in river management and pollution studies. *Zeitschrift für Geomorph* **56** (2012) 93.
15. Komorsky-Lovrić Š, Lovrić M. Theory of square-wave voltammetry of two electron reduction with the intermediate that is stabilized by complexation. *Electrochim Acta* **69** (2012) 60.
16. Kwokal Ž, Sarkar SK, Frančišković-Bilinski S, Bilinski H, Bhattacharya A, Chatterjee M. Mercury concentration in sediment cores from Sunderban mangrove wetland, India. *Soil Sediment Contam: Int J* **21** (2012) 525.
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33. Plavšić M, Strmečki S, Dautović J, Vojvodić V, Olujić G, Ćosović B. Characterization and distribution of organic matter using specific physico-chemical methods: a case study of the southeast Adriatic continental and shelf slope (Albania). *Cont Shelf Res* **39/40** (2012) 41.
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35. Ivošević DeNardis N, Žutić V, Svetličić V, Frkanec R. Adhesion signals of phospholipid vesicles at an electrified interface. *J Membrane Biol* **245** (2012) 573.
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37. Pletikapić G, Berquand A, Mišić Radić T, Svetličić V. Quantitative nanomechanical mapping of marine diatom. *J Phycol* **48** (2012) 175.

REVIEW ARTICLE

1. Udiković-Kolić N, Scott C, Martin-Laurent F. Evolution of atrazine-degrading capabilities in the environment. *Appl Microbiol Biotechnol* **96** (20 12) 1175.

BOOKS

1. Komorsky-Lovrić Š. 33 guidelines: Adsorptive accumulation, Background current, Marko Branica etc. In “Electrochemical Dictionary”, 2nd, Revised and Extended Edition. Bard AJ, Inzelt G, Scholz F (eds). Berlin, Germany: Springer, 2012. pp 20-967.
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3. Urbani R, Sist P, Pletikapić G, Mišić Radić T, Svetličić V, Žutić V. Diatom Polysaccha-

rides: Extracellular Production, Isolation and Molecular Characterization. In: The complex world of polysaccharides. Karunaratn DN (ed.) InTech, 2012 pp 345-367.
4. Ivanda M, Ivošević DeNardis N, Đerek V (eds), 2nd Adriatic School on Nanoscience, Nanoscience from Synthesis to Characterization, 2012, ISBN 978-953-6690-94-7
5. Hozić A, Vuletić T (eds), Book of Abstracts of the 11th Greta Pifat Mrzljak International School of Biophysics: Biomolecular Complexes and Assemblies, 2012.

Center for Marine Research

http://www.irb.hr/en/cim

DIVISIONAL ORGANISATION

Head: Nenad Smodlaka

The Centre for Marine Research consists of the following laboratories:

- Laboratory for marine molecular toxicology, Renato Batel
- Laboratory for marine ecotoxicology, Nevenka Bihari
- Laboratory for biomineralization nanostructure and radioecology, Davorin Medaković
- Laboratory for marine microbial ecology, Mirjana Najdek
- Laboratory for processes in the marine ecosystem, Robert Precali
- Laboratory for ecology and systematics of benthos, Ana Travizi

OVERVIEW OF THE DIVISION

The mission of the Center for Marine Research is the multidisciplinary study of processes in the marine environment from the subcellular to regional scale, especially in planktonic and benthic communities of the northern Adriatic Sea. In addition to basic research, the Center is involved in monitoring the Adriatic Sea for government purposes and as part of several international projects dedicated to protection of the marine environment.

TOP ACHIEVEMENTS

Seasonal fatty acid profile analysis to trace origin of food sources of four commercially important bivalves

Knowledge of bivalve food sources has great importance in aquaculture areas where cultured species usually occur at higher densities than in natural populations. Food sources were investigated by analyzing the fatty acid profiles in the digestive gland and muscle tissues of the European flat oyster Ostrea edulis and the black mussel Mytilus galloprovincialis, cultured in the water column, and the bearded horse mussel Modiolus barbatus and Noah's ark shell Arca noae from natural populations. Digestive gland fatty acid analysis revealed that during periods of higher plankton abundance in spring and summer, all species ingested mainly phytoplankton followed by zooplankton and detritus. During low plankton abundance in the autumn-winter period, zooplankton and/or detritus became more important in the bivalve diet. Fatty acid composition of muscle tissue indicated differences in selective incorporation of polyunsaturated fatty acid (PUFA) from their diets. While A. noae and M. barbatus significantly accumulated PUFAs during

all periods, O. edulis did so only during the spring-summer period. In M. galloprovincialis this tendency was not observed at all, suggesting better utilization of ingested food in bottom-dwelling species. Aquaculture in Mali Ston bay depends wholly on natural spatfall. This suggests that larviphagy, observed for all species, might constitute a self-regulating restriction to natural and/or commercial population growth (Ezgeta-Balić et al., 2012).

Changes in the planktonic community structure related to trophic conditions: a case study of the northern Adriatic Sea

Differentiation of the plankton food web structure was studied during the 2003-2008 period, in situations when the system of the northern Adriatic Sea switched from a low nutrient to higher nutrient regime. The biomass distribution between autotrophs, bacteria, protozoans and metazoans showed that within the upper part of the water column the microbial food web was developed during the stratification period (May-September) in oligotrophic conditions, with a larger heterotrophic/autotrophic (H/A) ratio in the western (1.4-1.7) relative to the eastern part (1.2-1.5). Classical food web patterns (H/A 0.3-0.7) were observed when additional nutrient supply by freshwater (stratification period) and/or by mixing throughout the water column (November-March) occurred. While the stratification period with freshets (originating from the Po River outflow) was characterized by an increased biomass of autotrophs and heterotrophs, there was a reduction of biomasses during the mixing period, indicating increased carbon export from the area. In the bottom layer, heterotrophs were not able to use the excess of autotrophic production, hence probably a part of the autotrophs sank to the sediments fuelling benthic communities. Moreover, recurrently higher metazoan biomass ratios relative to protozoans suggested the occurrence of herbivorous and microbial grazing modes in metazoans (Fuks et al., 2012).

Survival mechanisms of phytoplankton in conditions of stratification induced deprivation of orthophosphate: Northern Adriatic case study

Mechanisms by which phytoplankton adapted to PO_4 deprivation during the summer stratification in the northern Adriatic were studied. In the upper, more productive waters, phytoplankton induced high alkaline phosphatase activity (APA) to obtain phosphorus from the dissolved organic pool, and the P turnover time mediated by phytoplankton APA was very short (2 min-1.5 h). High affinity enzymatic activity combined with high hydrolysis rates allowed for metabolic flexibility of phytoplankton in this heterogeneous and fluctuating environment. Another possible mechanism of adaptation to the PO_4 deficit during the summer was a shift towards smaller cells. The smaller nanophytoplankton, supported by higher surface: volume ratios, is presumably able to produce more alkaline phosphatase, an exoenzyme bound to the cell surface. The progressive decrease in large cells and increase of smaller cells in the phytoplankton community during the summer supported this hypothesis. In upper waters with low PO_4 concentrations, phytoplankton reduced their P demand by a preferential synthesis of non-phospholipids. In bottom waters phytoplankton abundance was markedly lower than in upper waters and growth was probably light limited. In these deeper waters with higher PO_4 concentrations, phytoplankton did not use APA to obtain phosphorus and were able to synthesize more phospholipids. In deeper waters growth of bigger cells was favored (Ivančić et al., 2012).

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Unusual crystal formation in organisms - exceptions that confirm biomineralization rules

Marine organisms have been commonly used as bio-indicators of changes in the ma-

rine environment. Bioaccumulation of metals and lipophilic organic compounds through extraction from sea water is typically confirmed by chemical analysis of soft tissue. In this project unusual biominerals, influenced by unexpected environmental events, and caused by anthropogenic activity in several groups of marine organisms as well as freshwater and subterranean snails were presented with the aim of explaining how complex and sentinel mechanisms regulate environmental and physiological functions in mollusks. The analysis of hard structures consisting of biominerals can provide additional information on toxic element concentration, understanding of the biomineralization process and environmental evaluation (Medaković and Popović 2012; Pavat et al., 2012).

Molecular cross-talk between sponge host and associated microbes

Marine organisms, especially those that have a sessile lifestyle, such as sponges, are well known to have specific relationships with a great variety of microorganisms including bacteria and fungi. As the most simple metazoan phylum, the Porifera, which emerged first from a common ancestor during the transition from the non-Metazoa to the Metazoa, contain a wide array of recognition molecules, both for Gram-negative bacteria and for Gram-positive bacteria as well as for fungi. They react specifically with effector molecules to inhibit or kill the invading microorganisms. The elicitation and the subsequent effector reactions of sponges towards these microbes are outlined. In addition to the elimination of bacteria and fungi, some of these taxa are maintained as sponge symbionts, allowing them, for example, to accumulate the essential element manganese or to synthesize carotinoids. Sponges produce low-molecular-weight bioactive compounds and secondary metabolites, to eliminate microorganisms. In addition, they are armed with cationic antimicrobial peptides allowing them to defend against invasive microorganisms and, in parallel, to kill or repel metazoan invaders. The broad range of chemically and functionally different compounds qualifies the Porifera as the most important animal phylum to be exploited as a source for the isolation of new potential drugs. Initial molecular biological strategies have been outlined to obtain such compounds in a sustainable way, by recombinant production (Wang et al., 2012).

Structural and functional characterization of ribosomal protein gene introns in sponges

Ribosomal protein genes (RPGs) are a powerful tool for studying intron evolution. They exist in all three domains of life and are highly conserved. Accumulating genomic data suggest that RPG introns in many organisms abound with non-protein-coding-RNAs (ncRNAs). These ancient ncRNAs are small nucleolar RNAs (snoRNAs) essential for ribosome assembly. They are also mobile genetic elements and therefore probably important in the diversification and enrichment of transcriptomes through various mechanisms such as intron/exon gain/loss. snoRNAs in basal metazoans are poorly characterized. We examined 449 RPG introns, in total, from four demosponges: Amphimedon queenslandica, Suberites domuncula, Suberites ficus and Suberites pagurorum and showed that RPG introns from A. queenslandica share position conservancy and some structural similarity with “higher” metazoans. Moreover, our study indicates that mobile element insertions play an important role in the evolution of intron size. In four sponges 51 snoRNAs were identified. The analysis showed discrepancies between the snoRNA pools of orthologous RPG introns between S. domuncula and A. queenslandica. Furthermore, these two sponges show as much conservancy of RPG intron positions between each other as between themselves

and humans. Sponges from the Suberites genus show consistency in RPG intron position conservation. However, significant differences in some of the orthologous RPG introns of closely related sponges were observed. This indicates that RPG introns are dynamic even within shorter evolutionary time scales (Perina et al., 2012).

Silicateins, silicatein interactors and cellular interplay in sponge skeletogenesis: Formation of glass fiber-like spicules

Biomineralization processes are characterized by controlled deposition of inorganic polymers/minerals mediated by functional groups linked to organic templates. One metazoan taxon, the siliceous sponges, has utilized these principles and even gained the ability to form these polymers/minerals by an enzymatic mechanism using silicateins. Silicateins are the dominant protein species present in the axial canal of the skeletal elements of the siliceous sponges, the spicules, where they form the axial filament. Silicateins also represent a major part of the organic components of the silica lamellae, which are cylindrically arranged around the axial canal. With the demosponge Suberites domuncula as a model, quantitative enzymatic studies revealed that both the native and the recombinant enzyme display the same biosilica-forming activity in vitro as the enzyme involved in spicule formation in vivo. Monomeric silicatein molecules assemble into filaments via fractal intermediates, which are stabilized by the silicatein-interacting protein silintaphin-1. In addition to the silicateins, a catabolic silica-degrading enzyme, silicase, has been identified. Growth of spicules proceeds in vivo in two directions: first, by axial growth, a process that is controlled by evagination of cell protrusions and mediated by the axial filament-associated silicateins; and second, by appositional growth, which is driven by the extraspicular silicateins, a process that provides the spicules with their final size and morphology. This radial layer-by-layer accretion is directed by organic cylinders that are formed around the growing spicule and consist of galectin and silicatein. The cellular interplay that controls the morphogenetic processes during spiculogenesis is outlined. Silicateins are sponge-specific enzymes that facilitate silica polycondensation, resulting in biosilica formation. Biosilica represents the scaffold for the skeletal elements of the sponges, the spicules. The genes/cDNAs for the silicateins and the silintaphins are known. This review summarizes the characteristics of these proteins as well as the regulatory network underlying the formation of one of the most intricately structured skeletal structures of Metazoa, the siliceous spicules (Wang et al., 2012).

Mutual protection of ribosomal proteins L5 and L11 from degradation is essential for p53 activation upon ribosomal biogenesis stress

Impairment of ribosomal biogenesis can activate the p53 protein independently of DNA damage. The ability of ribosomal proteins L5, L11, L23, L26, or S7 to bind Mdm2 and inhibit its ubiquitin ligase activity has been suggested as a critical step in p53 activation under these conditions. Here, we report that L5 and L11 are particularly important for this response. Whereas several other newly synthesized ribosomal proteins are degraded by proteasomes upon inhibition of Pol I activity by actinomycin D, L5 and L11 accumulate in the ribosome-free fraction where they bind to Mdm2. This selective accumulation of free L5 and L11 is due to their mutual protection from proteasomal degradation. Furthermore, the endogenous, newly synthesized L5 and L11 continue to be imported into nucleoli even after nucleolar disruption and colocalize with Mdm2, p53, and promyelocytic leukemia protein. This suggests that the disrupted nucleoli may provide a platform for L5- and L11-dependent p53 activation, implying a

role for the nucleolus in p53 activation by ribosomal biogenesis stress. These findings may have important implications with respect to understanding the pathogenesis of diseases caused by impaired ribosome biogenesis (Bursać et al., 2012).

Toxin-producing Ostreopsis cf. ovata are likely to bloom undetected along coastal areas

Mass appearances of the toxic dinoflagellate genus *Ostreopsis* are known to cause dangerous respiratory symptoms in humans exposed to their aerosols. The outbreaks can appear in shallow marine waters of temperate regions around the globe. We followed a massive bloom event at a public beach on the northern Adriatic coast near Rovinj, Croatia. We identified the responsible species and the produced toxins as well as the dynamics of the event with respect to environmental conditions. *Ostreopsis* cf. *ovata* appeared en mass from September through October 2010 at a public beach near Rovinj, Croatia but remained undetected by public health organizations. Respiratory symptoms were observed whenever humans were exposed to substrate samples containing large numbers of *Ostreopsis* cells. At times of mass abundance of *O.* cf. *ovata* exposure to aerosols on the beach evoked respiratory symptoms in humans. Our measurements showed high cell abundances and high toxin contents with a stable relative contribution of putative Palytoxin and Ovatoxins a-e. Artificial beach structures proved to dramatically reduce settling of the observed *Ostreopsis* biofilm. Blooms like those reported herein have a high potential to happen undetected with a high potential for affecting the health of coastal human populations. Increased monitoring efforts are therefore required to understand the ecology and toxicology of these bloom events and reduce their negative impact on coastal populations (Pfannkuchen et al., 2012).

Comparison of bioaccumulation and biomarker responses in Dreissena polymorpha and D. bugensis after exposure to resuspended sediments

The zebra mussel *Dreissena polymorpha* is widely used as a sentinel organism for the assessment of environmental contamination in freshwater environments. However, in the River Rhine (Germany), the *D. polymorpha* population is declining, whereas the closely related quagga mussel *D. bugensis* is found in high numbers at some sites. In the present laboratory study, *D. polymorpha* and *D. bugensis* were exposed to resuspended native sediments for 2 weeks. Wet sediments (<63 ?m, 100 mg l -1 dry weight) were used as surrogate suspended particulate matter to mimic one of the mussels' main uptake route for chemicals. The sediments were sampled in (1) the River Elbe in Dessau, a site known to be highly polluted with, e.g., organochlorine (OC) pesticides and (2) at a relatively unpolluted site in Havelberg on the River Havel, one of the Elbe's tributaries. Chemical analysis of persistent OC compounds (seven polychlorinated biphenyls [PCBs], DDT and its metabolites (DDX), hexachlorocyclohexanes [HCHs], and hexachlorobenzene [HCB]) in soft tissue of mussels showed significantly greater values of PCBs 101, 118, 153, 138, 180, the sum of seven PCBs, and p,p'-DDD in *D. bugensis* compared with *D. polymorpha*. Fourteen days of exposure to the Dessau sediment increased the concentration of p,p'-DDE and p,p'-DDD, as well as the sum of DDX, in both species compared with the Havelberg sediment. Interspecific differences were less pronounced when we compared chemical concentrations with lipid content instead of dry-weight of tissue because *D. bugensis* had greater levels of total lipid than *D. polymorpha*. DNA damage in gills, as measured with the comet assay, was greater in *D. bugensis* compared with *D. polymorpha*. Simultaneously, the content of heat-shock protein (hsp70) in gills was great-

er in *D. polymorpha* than in *D. bugensis*. DNA damage and hsp70 were not induced by exposure time or sediment type. This study shows that *D. bugensis* and *D. polymorpha* may differ in their bioaccumulation potential for OC pesticides as well as their levels of DNA damage and hsp70. Therefore, more studies are needed before the quagga mussel can be used as an alternative test organism (Schaefer et al., 2012).

Diversity, occurrence, and habitats of the diatom genus Bacteriastrum (Bacillariophyta) in the northern Adriatic Sea, with a description of the novel species B. jadranum

Ongoing phytoplankton monitoring programs over the last 12 years in the northern Adriatic Sea have shown that the diatom genus *Bacteriastrum* is an important component of the pelagic diatom assemblage. The main goals of this study were to identify which *Bacteriastrum* species occur in the northern Adriatic Sea and describe their distributions. *Bacteriastrum comosum* and *B. hyalinum* f. *princeps* were rare, while *B. delicatulum* , *B. hyalinum* , and *B. mediterraneum* were frequently present, together with the newly proposed species *B. jadranum* , described herein. This new species is weakly silicified and is mainly characterized by a large aperture between each cell of the filament. Cells are connected to each other by 8 – 12 setae, which cross at a distance equivalent to the diameters of 2 – 3 cells. There is no difference in the orientation of the setae on the two terminal cells, hence the species is placed in the section *Isomorpha*. The new species was recorded throughout the study area, in both coastal and offshore waters, with higher cell abundances in the vicinity of the Po River during the September – October period. The maximum cell abundance of *B. jadranum* was 244.2 × 10^3 cells l^{-1} in the surface waters at 44.75666667°N, 12.75°E in September 2006, sometimes representing up to 46 % of the entire phytoplankton assemblage, as recorded in the surface waters at 45.06833333°N, 13.515°E in October 2008 (Godrijan et al., 2012).

Predictability of northern Adriatic winter conditions

Geostrophic circulation patterns in the northern Adriatic winters of 2000 and 2001 have been analysed on the basis of a large amount of data collected within the large international project Processes of mucilage formation in the Adriatic and Tyrrhenian seas: monitoring of the profile Rovinj-Po River delta (Mucilage formation in the Adriatic and Tyrrhenian seas - MAT). While in the winter of 2001 the waters of the Po River were drawn offshore into the northern Adriatic, in 2000 they remained close to the coast. Differences in winter circulation patterns were induced by processes occurring during the previous autumn, pointing to the fact that a forecast of the winter northern Adriatic conditions is possible several months in advance. Studies of the winter northern Adriatic conditions are important as the presence of Po River water impacts the organic production of the entire region (Supić et al., 2012).

Fluctuations and trends in northern Adriatic marine systems: from annual to decadal variability

Numerous studies in a long term series on river discharges, oceanographic features, plankton, fish and benthic compartments, collected since the 1970s have revealed significant changes of mechanism and trophic structures in northern Adriatic ecosystems. Based on a series of relevant data (1972-2010) collected at oceanographic stations along the profile Rovinj-Po Delta (RV001, SJ101-SJ108) the mechanism of long-term changes in the trophic status of the northern Adriatic was studied. A systematic trend of oligotrofication following 2002, especially pronounced in the western part of the region, was established. This trend is caused by

the extremely low flow of the river Po, especially in the spring, as well as increased frequency of intrusion of middle Adriatic water. Climatic and oceanographic changes in the eastern northern Adriatic were reflected in phytoplankton abundance, community composition and seasonal cycle alternations with especially prominent changes in the *Pseudo-nitzschia delicatissima* and *Pseudo-nitzschia seriata* groups. Presumably, similar changes occurred in the entire Adriatic as well (Djakovac et al., 2012; Giani et al., 2012; Marić et al., 2012).

EDUCATION

The Center is involved in the organisation of Marine Sciences Studies (undergraduate) at the Juraj Dobrila University and in the Polytechnics, High technical school in Pula. The majority of courses are organized by the Center's scientists. Undergraduate and postgraduate courses were given at the Universities of Zagreb (Faculty of Science), and in PhD study Molecular Biosciences organized by Ruđer Bošković Institute and Universities of Osijek and Dubrovnik.

PROJECTS

Research projects supported by the Ministry of Sciences, education and Sport

1. Impact of pollution on programmed biosynthesis in marine invertebrates, Renato Batel
2. Ecotoxic effect of contamination on marine organisms, Nevenka Bihari
3. Biomineralization processes in marine organisms, Davorin Medaković
4. Structure and physiology of microbial communities in northern Adriatic front, Mirjana Najdek
5. Mechanisms of long-term changes in the northern Adriatic ecosystem, Robert Precali
6. Biodiversity of benthic communities in the Adriatic: natural and human impacts, Ana Travizi
7. Croatian national monitoring programme "Systematic research of the Adriatic Sea as a base for sustainable development of the Republic of Croatia" (Project "Adriatic"), Nenad Smodlaka

Organization of conferences, congresses and meetings

1. "Biodiversity" workshop for project „Providing Access to the Phytoplankton Biodiversity of the Northern Adriatic Sea: Taxonomy, Systematics, Genetics, Ecology and Open Access Data Management" Rovinj, 21.9-6.10.2012.
2. "Biomintec" Marie Curie Workshop, Zagreb, 22.-24.08.2012.

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2. Ezgeta-Balić D, Najdek M, Peharda M, Blažina M. Seasonal fatty acid profile analysis to trace origin of food sources of four commercially important bivalves. *Aquaculture* **334** (2012) 89.
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4. Fuks D, Ivančić I, Najdek M, Lučić D, Njire J, Godrijan J, Marić D, Šilović T, Paliaga P, Blažina M, Precali R, Orlić S. Changes in the planktonic community structure related to trophic conditions: the case study of the northern Adriatic Sea. *J Mar Syst* **96/97** (2012) 95.
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8. Marić D, Kraus R, Godrijan J, Supić N, Djakovac T, Precali R. Phytoplankton response to climatic and anthropogenic influences in the north-eastern Adriatic during the last four decades. *Estuar Coast Shelf Sci* **115** (2012) 98.
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10. Perina D, Korolija M, Mikoč A, Roller M, Pleše B, Imešek M, Morrow C,Batel R, Ćetković H. Structural and functional characterization of ribosomal protein gene introns in sponges. *PLoS ONE* **7** (2012) e42523.
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12. Schäfer S, Hamer B, Treursić B, Möhlenkamp C, Spira D, Korlević M, Reifferscheid G, Claus E.Comparison of bioaccumulation and biomarker responses in *Dreissena polymorpha* and *D. bugensis* after exposure to resuspended sediments. *Arch Envir Cont Toxicol* **62** (2012) 614.
13. Supić N, Kraus R, Kuzmić M, Paschini E, Precali R, Russo A, Vilibić, I. Predictability of northern Adriatic winter conditions. *J Mar Syst* **90** (2012) 42.
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Centre for Informatics and Computing

CIR

http://www.irb.hr/en/cir

ORGANISATION OF THE CENTRE

Head: Karolj Skala

The Centre for Informatics and Computing Science (CIR) consists of the following units:

- Optoelectronics and Visualisation Laboratory,
- Department for R&D of ICST systems,
- Department for Information systems,
- IT Services Department

centar za informatiku i računarstvo

OVERVIEW OF THE CENTRE

The mission of the Centre is to become a leading ICST (Information Communication Science Technology) centre for the research, development and implementation of new computing, visualisation and information processing paradigms and techniques. The Centre works to enable scientific dissemination and application of these techniques across a broad spectrum of scientific disciplines. The Centre supports multidisciplinary and multi-institutional scientific work based on the eScience platform and through Virtual Organizations at the national and global level. As part of the European Research Area we actively participate in national and EU projects. CIR scientists are working on the AdriaScience gateway, CloudMan and Galaxy, HPC and Cloud oriented projects with the goal of establishing infrastructure for complex problem solving based on eScience technologies. The Center provides technical and technological support and maintains basic information services at RBI on the Linux platform.

TOP ACHIEVEMENTS

EU FP7 DARIAH project become to ERIC

The ESFRI project DARIAH received a positive evaluation response from the European Commission in the first stage of the application process to become a member of the European Research Infrastructure Consortium, DARIAH ERIC. Following the successful revision of DARIAH, submission of a formal request to establish the European organization was made.

Cloudmen implementation at the University of Melburne

Our collaboration with the University of Melbourne on the eCloudMan project proposal continued with the Genomics Virtual Laboratory (GVL) project which is a combination of scalable computer infrastructure, workflow platforms and community resources for genomics researchers. At this stage, the GVL comprises: a prototype workflow management system based on the Galaxy framework, a bioinformatics toolkit (for command-line users) based on CloudBioLinux, and a visualisation service based on the UCSC Genome Browser, all implemented on the Australian national research cloud (NeCTAR). In addition, the GVL is developing a set of tutorials and exemplar protocols targeted at common high throughput genomics tasks. CloudMan is an application that is being continuously developed at RBI and has provided an excellent basis for establishing a set of required cloud services for the GVL and other users at the global level.

New EU FP7 project

Work has begun on the new *Embedded Computer Engineering Learning Platform*-E2LP project. This platform will facilitate the novel development of a universal approach in the creative learning environment and knowledge management areas that encourage use of ICT. The new learning model is challenging the education of engineers in embedded systems design through real-time experiments that stimulate curiosity with the ultimate goal to support students in their acquisition and understanding of personal conceptual knowledge based on experiments. In addition to the technological approach, the use of cognitive theories on how people learn will help students to achieve a stronger and smarter adaptation of the subject. The applied methodology will be evaluated from the scientific point of view in parallel with the implementation in order to feed back results to R&D.

COST IC0805 project

CIR has become part of the *Open European Network for High Performance Computing on Complex Environments* COST IC0805 action. Across different fields of science and engineering we have solved complex and challenging problems with homogeneous high performance computers. Nowadays, the emergence of heterogeneous computing allows research groups, enterprise and educational institutions to use networks of processors already available. Research achievements were presented at a workshop organized by the COST Action IC0805 in Genova, Italy. We closely collaborated with the research group from University Jaume I, Castellon (Spain) on this project.

Data flow computing initiatives

The Centre joined with the Maxeler MAX-UP university program and provided access to the Data Flow Computing architecture that will be used to address the Big Data problem of assembly; active research in HPC and Cloud computing and development of novel DNA assembly algorithms. We established a formal collaboration with the European Bioinformatics Institute on Data Flow Computing applications.

Dynamic 4D Thermography Imaging System

We developed a novel concept for the standardisation of human body 3D thermal models, captured by multi-resolution real-time 3D thermal imaging system. The standardisation procedure consists of four different processes: Skeleton Detection, Skeleton Transformation, Vertex Deformation and Thermal Texture Mapping process. The presented concept of 3D thermal model standardisation enables novel and practical methods for model comparison and analysis.

NEW EQUIPMENT

New equipment from CIR R&D activity advanced Dynamic 4D themography Imaging System.

PROJECTS

Research programs supported by the Ministry of Sciences, Education and Sport

1. Distributed Computing and Visualisation, Karolj Skala

Research projects supported by the Ministry of Sciences, Education and Sport

1. Scientific Visualisation Methods, Karolj Skala

Research projects supported by the EU

1. Embedded Computer Engineering Learning Platform-E2LP, EU FP7, Karolj Skala
2. Application Information Services for Distributed Computing Environments AIS-DC, EU, FP7, Karolj Skala, Enis Afgan
3. SCIentific gateway Based User Support, SCI-BUS, EU FP7, Karolj Skala

EDUCATION

CIR provides doctoral courses at the Faculty of Electrical Engineering and Computing and Faculty of Graphical Arts at the University of Zagreb and the University Josip Jurja Strossmayer in Osijek, Bussiness Management at the High Scool „Baltazar Adam Krčelić“ in Zaprešić.

AWARDS

Silver medal ARCA, 10th International exhibition of inventions for 4D thermographic system, October 13, 2012.

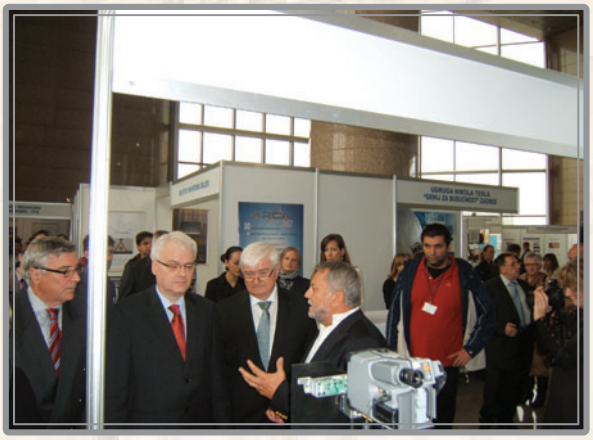

Fig. 4D Thermovision System at ARCA 2012.

ORGANIZED CONFERENCES, WORKSHOPS AND SUMMER SCHOOLS

1. 35th International Convention MIPRO, CONFERENCE on DISTRIBUTED COMPUTING AND VISUALISATION SYSTEMS (DC VIS), Opatija, Croatia, May 23-25, 2012
2. Research Infrastructure Disemination Event, RIDE 2012, Opatija, May 21-24, 2012
3. “Galaxy CloudMan.” Workshop at Galaxy Community Conference 2012, Chicago, USA, July 2012 (Afgan, Enis)
4. “GVL Galaxy Workshop.” Workshop at eResearch Australasia 2012, Sydney, Australia, November 2012 (Afgan, Enis)
5. SCI-BUS Summer School, Budapest, Hungary, July 2-6, 2012 - Scientific gateways and scientific workflow repositories, organized by the SCI-BUS EU FP7 project
6. SCI-BUS code camp, Budapest, Hungary, September 28-30, 2012 - Code camp for the SCI-BUS gateway and application developers, organized by the SCI-BUS EU FP7 project.

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2. Bojić I, Lipić T, Podobnik V. Bio-inspired clustering and data diffusion in machine social networks. In: Computational social networks: mining and visualization. Abraham A (ed.). London, Springer Verlag, 2012. pp. 51-79.

Centre for Nuclear Magnetic Resonance

http://www.irb.hr/en/nmr

ORGANIZATION OF THE CENTRE

Head: Dražen Vikić-Topić (Vilko Smrečki until May 23, 2012)

The NMR Centre consists of the following laboratories:

- Laboratory for NMR spectroscopy and modelling, Dejan Plavšić
- Glass Laboratory, Andrea Moguš-Milanković

OVERVIEW OF THE CENTRE

The Centre carries out scientific research in NMR spectroscopy in the fields of inorganic, organic and bioorganic chemistry, and provides its scientific services to the whole academic community of the Republic of Croatia. The Centre also provides educational and professional support to researchers from governmental institutions and the pharmaceutical industry, as well as participating in higher education at the Universities of Zagreb, Rijeka, Split and Osijek. Equipment in the Centre includes Bruker Avance 300 and 600 MHz NMR spectrometers as well as a Varian Gemini 300 MHz NMR spectrometer located at the Faculty of Pharmacy and Biochemistry of the University of Zagreb.

The Laboratory for NMR Spectroscopy and Modelling performs experimental and theoretical research on organometallic and bioorganic compounds, in photochemistry and food chemistry as well as mathematical chemistry and modelling, with the aim of identifying bioactive compounds, their structures and properties/activities relationships. The Glass Laboratory performs investigations on the electrical conductivity of super ionic glasses such as LiI-AgI-B2O3 doped with transition metal ions, as a potential electrolyte in lithium batteries. This research is directed toward development of new nano- and microcrystalline materials produced by induced controlled crystallization.

TOP ACHIEVEMENTS

Representation of proteins

We have introduced a novel graphical representation of proteins starting with construction of a map of a protein obtained from a matrix, the elements of which record the adjacencies of pairs of amino acids in the primary structure of a protein. The construction

of protein binary codes that can serve as protein descriptors has been proposed (Randić M, et al., 2012).

NMR structure determination

The photochemical behaviour of some novel dithiophene and dibenzothiophene derivatives were studied by NMR at low concentrations (Vuk D, et.al., 2012). Novel bioactive complexes of nickel(II), zinc(II), cadmium(II) and mercury(II) have been elucidated by X-ray and ^{1}H and ^{13}C NMR (Đaković M, et.al., 2012).

Food chemistry

Intensive computational investigations of the structure and activity of the antioxidant compound morin and the dominant anion of morin were performed by DFT and semiempirical PM6. Results indicate that the 4'-OH group of 2'-O^- phenoxide anion is the active site for radical inactivation at physiological pH. The faster, semiempirical PM6 method compares favourably with the more accurate and time consuming DFT method (Marković Z, et.al., 2012).

Modulation of hepatoprotection by means of an antisense peptide

We have found that short peptides can be applied to immunochemical assays and analysis, which opens up the possibility of applying the described procedures as a substitute/supplement to monoclonal antibodies in the diagnosis and prognosis therapy of neoplastic diseases as well as vaccine development (Bradamante M, et al., 2012).

Polaronic Mobility in Boron Doped Iron Phosphate Glasses: Influence of Structural Disorder on Summerfield Scaling

A detailed study of the internal strain that appears upon the addition of a second glass former and its effect on the relaxation processes in polaronic glasses revealed a deviation of the common scaling curve. The origin of this behaviour is a local structural disorder caused by structural changes in the early stage of B_2O_3 addition as well as at the initial incorporation of BO_4 tetrahedra into phosphate chains (Moguš-Milanković A, et al., 2012).

EDUCATION

Members of the NMR Centre are involved in teaching bachelor level courses at the University of Rijeka and the School of Dentistry, University of Zagreb, PhD level courses at the Faculty of Science and the School of Medicine, University of Zagreb, in joint international doctoral courses through the University of Rijeka, Glaxo/Smith/Kline and Ruđer Bošković Institute, joint PhD courses through the Ruđer Bošković Institute and University of Osijek and University of Dubrovnik, Faculty of Medicine University of Rijeka and at the Faculty of Science University of Split. NMR members also supervised 5 PhD theses through the University of Zagreb.

PROJECTS

Research projects supported by the Ministry of Science, Education and Sports

1. NMR spectroscopy and modelling of bioactive molecules, Dejan Plavšić
2. Influence of structure on electrical properties of (bioactive) glasses/ceramics, Andrea Moguš-Milanković
3. Modelling of bioactive molecules and testing of their properties and activity, Nikola Štambuk
4. Developing methods for modelling properties of bioactive molecules and proteins, Bono Lučić

Bilateral projects

1. Investigation of relationships between structure and biological activity of polyphenols, bilateral Croatian-Serbian project, Bono Lučić

Other projects

1. Evaluation of new bioactive materials and procedures in restorative dental medicine (Croatian Science Foundation), Collaborative Research Programmes RBI-IF-School of Dentistry Zagreb, Programme leader: Z. Tarle, RBI project leader: A. Moguš-Milanković

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2. Randić M, Novič M, Choudhury RA, Plavšić D. On graphical representation of transmembrane proteins. *SAR QSAR Environ Res* **23** (2012) 327.
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8. Moguš-Milanković A, Pavić L, Ertap H, Karabulut M. Polaronic mobility in boron doped iron phosphate glasses: influence of structural disorder on summerfield scaling. *J Am Ceram Soc* **95** (2012) 2007**.**
9. Filipič C, Moguš-Milanković A, Pavić L, Karabulut M, Levstik A. Polarons in boron doped iron phosphate glasses. *J Non-Cryst Solids* **358** (2012) 2793.

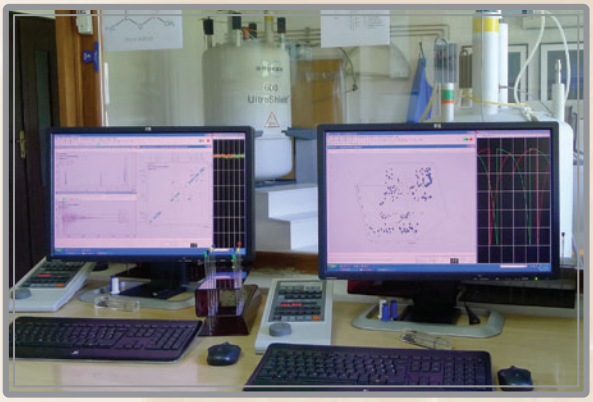


Fig. 1. a) ORTEP drawing with atom numbering of complex $[Ni(pia)_2(H_2O)_2](NO_3)_2$ confirmed by NMR spectroscopy in liquid phase (above). Crystal packing with hydrogen bonds (indicated by dotted lines) involving only the carboxamide (below).

b) The dependence of the dc conductivity, σdc, at 303 K and activation energy for dc conductivity, Ea, upon the heating temperatures (a). SEM micrographs of the zinc iron phosphate glass heat treated at 963 K (scale bar 1μm), inset: crack interior (b). Thermally induced formation of larger crystalline grains with size up to 500 nm, leads to appearance of better defined grain surfaces and interfacial disordered regions between grain boundaries and glassy matrix. In the interface regions which contain higher concentration of Fe^{2+}- Fe^{3+} pairs the conductivity is enhanced.

Library

http://library.irb.hr

Head of Library: Bojan Macan

OVERVIEW OF LIBRARY ACTIVITIES

Access to relevant scientific information is one of the stepping stones of successful scientific research and libraries play an important role in this process. New information technologies have changed the way in which scientists communicate among themselves and libraries have to follow these changes and change their role accordingly. The RBI Library has recognized the open access movement as the only path which will lead to the future development of scholarly publishing in the right direction and therefore it initiated numerous activities related to the open access movement and easier access to scientific information. In 2012 one of the main activities of the RBI Library was the release of the Full-text Institutional Repository of the Ruđer Bošković Institute (FULIR - http://fulir.irb.hr) as well as disseminating information on the open access initiative among researchers, as well as librarians. In September 2012 we participated as the national representative in the creation of the Minsk Recommendation for Open Access to Scientific Information document at a Regional Consultation on "Open Access to Scientific Information and Research – Concept and Policies" which was organized by UNESCO.

There are many benefits of open access for scientific information: the public has access to the results of scientific research financed with taxpayers' money; scientific institutions and their researchers increase their visibility while at the same time their work gains greater impact in the scientific community. Open access of scientific information in general contributes to the faster and more balanced development of science worldwide.

FULIR is an institutional repository of the Ruđer Bošković Institute in which RBI employees can archive full texts of all types of documents produced within their scientific research (full text of articles published in scientific journals, papers published in conference proceedings, graded papers, book chapters, monographs, various reports, presentations and posters presented at conferences), as well as audio-video material and original research data (datasets). The main idea behind FULIR is to gather together the whole of RBI's scientific output (published and unpublished) and to present it in open access to the public. Depending on the selected options and copyright issues records stored in the repository are visible to everyone, only to registered users, or only to system administrators. It is also possible for certain full text documents to implement an access embargo for a specified period of time. Logging in to the system is done through an AAI user identity after which the user can start depositing bibliographic information and uploading full texts of documents.

In order to establish this institutional repository the RBI Library has already digitized a collection of old photographs, which is available in the Photo gallery, as well as collections of the RBI Annual Report (all available reports since 1955), and *Rudjer* – the Institute's newsletter (all available editions since 1994). FULIR was presented to the public in October 2012, as part of the celebration of International Open Access Week and the 102nd Library Colloquia.

Figure 1. The Full Text Institutional Repository of the Ruđer Bošković Institute - FULIR

COLLECTION DEVELOPEMENT

In 2012 RBI scientists had access to more than 42.000 free and fee journals, around 30 free and fee biomedical and natural sciences databases, as well as 42 biomedical e-books. However, access to current issues of journals was not always possible. In addition to subscriptions at the Croatian academic consortia level and open access journals, the Library subscribed to 243 journals (subscription to selected titles from different publishers, as well as to journals packages from IOP and Emerald). Quick access to all available journals was provided via the Pero search engine (http://knjiznica.irb.hr/pero/) as well as through EZB Elektronische Zeitschriftenbibliothek (http://lib.irb.hr/web/hr/casopisi/item/202-ezb.html).

In 2012 the Library acquired only 102 new books, due to a reduction in our overall budget. An additional 125 books were donated to the Library, mainly from the Sabre Foundation's Book Donation Program (88 books). Since 1986, Sabre has helped to fill the need for high quality, educational materials in developing countries and countries in transition, with more than 80 countries benefiting from this work. Over 200 publishers have participated in Sabre's Donation Program. Sabre's practical work to promote education and free inquiry stems from its philosophical programs, directed for the past 25 years by Josiah Lee Auspitz. After more than a quarter of a century of supporting education around the world, the Sabre Donation Program is coming to an end. Additionally, RBI researchers donated 11 books to the collection of publications written or edited by RBI researchers, which are part of the permanent exhibition in the Library reading room in the 5th wing. Five new books were acquired for the special collection of publications about Ruđer Bošković.

In the period from May to the end of December the Library conducted a books inventory. During the inventory, all books were marked with barcodes ensuring a faster, au-

Figure 2. 'Take it or leave it' – book exchange organized on the lawn in front of the first wing at RBI

tomated process of book circulation in the future. A total of 466 books were written off, leaving 24.319 books remaining in the library holdings. Thanks to the integrated library system – Koha, the inventory process was much easier and faster than in previous years.

During 2012 the Library also organized two book exchanges , our "Take it or leave it" events. RBI employees could bring in their used books and exchange them for other books. The exchange in July was organized in the open (on the lawn in front of the first wing) and that event was very well received. The Winter exchange was held in the library reading room. In addition to books, people were also encouraged to bring in DVD's and magazines like National Geographic for the exchange. Through these events about 400 books were exchanged, and any remaining books were offered as donations to other libraries.

LIBRARY SERVICES

Interlibrary loan

The RBI library overcame the shortages of its collections through a well-established interlibrary loan and lending service with libraries from Croatia and abroad. In 2012 the RBI library received about 800 document delivery requests which were resolved, mostly free of charge, thanks to other Croatian libraries and to the well established network of EURASLIC/IAMSLIC libraries. In addition, the RBI library also received about 600 requests for document delivery from other Croatian libraries.

The In-house developed Oracle application SEND (Electronic Documents Acquiring System), has been active from 2003-2012 fulfilling more than 8000 requests from IRB staff, and more than 5000 requests from other Croatian libraries. SEND has now completed its „working life", opening the way to a new SEND application. The basic version of the new SEND application is already up and running, but its full version with new functionalities is still under development.

Bibliometric analysis

The Library has continued to provide bibliometric analysis, primarily for RBI scientists, and for other scientists requiring the different types of certificates that the Library offers. The Library issued various certificates for the purposes of promotion, project applications, scholarships etc. In 2012 the Library issued 130 citation certificates. The most requested certificates have been:

- certificates with the number of papers published in journals which are indexed in the Web of Science/Scopus/ Current Contents databases
- citation certificate of papers indexed in the Web of Science/Scopus databases
- certificate of the Journal Impact Factor for a given year

Different bibliometric analyses for various purposes are also provided for the whole Institute.

International cooperation

The Library continued its international cooperation with EURASLIC (European Association of Aquatic Sciences Libraries and Information Centers) and its parent organization IAMSLIC (European Association of Aquatic Sciences Libraries and Information Centres). Library staff had an active role in EURASLIC activities, as well as in its subgroup ECET (European Countries in Economic Transition). One member of the library staff is now a member of the EURASLIC Board (Executive secretary, website and newsletter editor), and one is a member of the IAMSLIC Strategic Planning Group.

Organization of events

The Library continued to organize the RBI Library Colloquia. Colloquia topics were cho-

sen to be of interest not only to librarians, but also to RBI staff and the general public. In 2012 five colloquia were organized. Two of these had a special theme:

- Jubilee 100th colloquia on June 13th – Since 1999, the Library has been hosting lecturers from Croatia and abroad, covering topics from information sciences, computer sciences, web and informatics, scientific communication and popular science. The 100th colloquium was celebrated with a special program which included ten short lectures. The main topic was new library services for new generations of library users, which attracted both colleagues from other libraries as well as RBI staff. RBI also supported and helped with the organization of this colloquium.
- 102nd colloquium during the International Open Access Week on October 25th – The program included a short lecture about open access in scientific publishing and official presentation of the RBI institutional repository FULIR.

Figure 3. Lectures at the jubilee 100th Library colloquium

The Library also actively participated in the event "The Bošković – Tesla Synergy", organized by RBI in December to mark the 70th anniversary of Nikola Tesla's death. In parallel with a sculpture exhibition at RBI, the Library organized a small exhibition of valuable books about or written by Nikola Tesla and Ruđer Bošković which are part of the Library's collection.

PROJECTS

Together with 41 European partners the RBI Library was involved in the 7th Framework Programme OpenAIREplus (2nd Generation of Open Access Infrastructure for Research in Europe), intended to facilitate access to the entire Open Access scientific production of the European Research Area, providing links from publications to data. As part of the project we plan to include Croatian peer reviewed scientific publications and associated datasets in the OpenAIRE portal and make them part of the collaborative networking structure.

In 2012 part of the Library staff was individually active in the FP7 project entitled *Support for Establishment of National/Regional Social Sciences Data Archives (SERSCIDA)*, which is charged with the development of digital archives of original research data in the field of social sciences.

In 2012 the Library continued to provide and monitor input to the Croatian Scientific Bibliography – CROSBI (http://bib.irb.hr) during which 21.513 new bibliographic records, many of them with full-text, were added. At the end of 2012 CROSBI included information on 355.610 research articles and other types of work written by Croatian researchers. The Library continued to maintain the *Who's Who in Science in Croatia* service (http://tkojetko.irb.hr), which has been used as the basis for collaboration with the publisher *Thomson Reuters* and the creation of *ResearcherID* for RBI researchers. *ResearcherID* integrates the publications from databases which are part of the Web of Knowledge interface and provides a solution to the author ambiguity problem within the scholarly research community. Unique identifiers enable researchers to manage their publication lists, track their citations and h-index, identify potential collaborators and avoid author misidentification. In addition, integration with *Who's Who in Science in Croatia* serves to improve the visibility of Croatian researchers.

Due to significant cuts in subscriptions, the Croatian Centre for Online Databases

(http://www.online-baze.hr) offered access to fewer databases than in previous years. Access to major publishers' databases such as *Thomson Reuters, Elsevier, EBSCO* and *Ovid* was provided in cooperation with the Croatian Ministry of Science, Education and Sports. A successful collaboration with the University Computing Centre at the University of Zagreb (SRCE) through the Portal of the Croatian scientific journals HRČAK (http://hrcak.srce.hr) resulted in access to more than 300 open access journals.

The lack of financial support in 2012 resulted in only minor changes to the interfaces, features and database structures of all of the above mentioned information services, and the support we got from students in the Department of Information Science at the University of Zadar was invaluable. In the future we will continue to work on major improvements integrating interoperability tools, monitoring tools and authority tools.

Figure 4. Library's FP7 projects - OpenAIREplus and SERSCIDA

EDUCATION

During 2012 the Library continued with its Short Educational Library Seminars – KEKS. The seminars consist of hour and a half or two hour workshops and short lectures (45 minutes). The seminars were held periodically in small groups. A total of twelve seminars with 83 participants were held in 2012.

Library staff were also involved in undergraduate and graduate level teaching at the University of Zagreb and University of Zadar.

AWARDS

Bojan Macan received the Croatian librarian association award Eva Verona for special dedication to work, innovation and promotion of librarianship in Croatia.

SELECTED LECTURE

1. Stojanovski J. Will (for-profit) scholarly publishing system transform open access movement? Annual Meeting of the Journal of Central European Agriculture international editorial bord, Zagreb, Croatia, October 10, 2012.
2. Macan B. Let us 'measure' our users - bibliometric analysis as library services. 100th colloquium of the Ruđer Bošković Institute Library, Zagreb, Croatia, June 13, 2012.
3. Stojanovski J. Institutional repositories - can they change the scholarly publishing system. 100th colloquium of the Ruđer Bošković Institute Library, Zagreb, Croatia, June 13, 2012.
4. Macan B. Back to future - services of modern libraries. Medical Information Conference Croatia (MICC) 2012, Zagreb, Croatia, June 15, 2012.
5. Stojanovski J. Open access: why, where and how? Publishing integrity in the digital age. Workshop for Journal Editors, University of Split, Split, Croatia, July 6-7, 2012.

SELECTED PUBLICATIONS

1. Macan B, Pikić A, Mayer, M. (Inter)national orientation of Croatian social sciences and arts and humanities journals indexed in the Web of Science database. Društvena istraživanja. **21** (2012), 505.
2. Stojanovski J. Supporting open access nationwide. The Fifth Belgrade International Open Access Conference Proceedings. Šipka P (ed.). Beograd, 2012, pp 75-87.
3. Stojanovski J. Analysis of academic library web sites for services. Libraries in the Digital Age (LIDA) Proceedings. Pehar F (ed.).

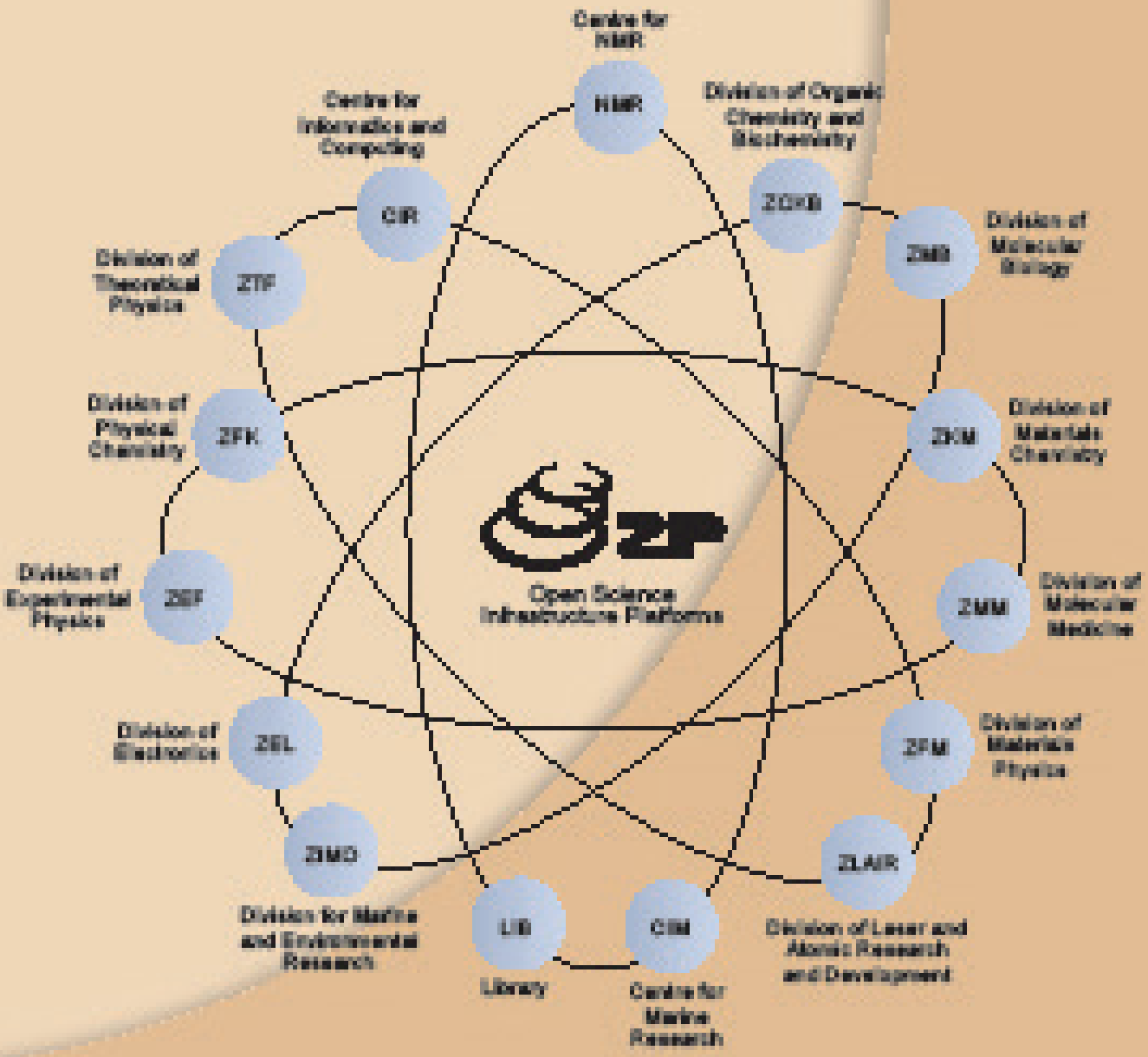
Zadar, Sveučilište u Zadru, 2012 (online edition).
4. Stojanovski J, Papić A. Quantitative indicators of academic libraries' involvement in educational process. Proceedings of the ITI 2012 34th International Conference on Information Technology Interfaces. Luzar-Stiffler V, Jarec I, Bekić Z (ed.). Zagreb, University Computing Center SRCE, University of Zagreb, 2012, pp 255-260.
5. Stojanovski J, Papić A. Information services in academic libraries: browsing services vs. searching services. Central European Conference on Information and Intelligent Systems CECIIS. Hunjak T, Lovrenčić S, Tomičić I (ed.). Varaždin, University of Zagreb, Faculty of Organization an Informatics, 2012, pp 85-90.
6. Pažur I. MENDELEY - a compass for navigating in the sea of scientific papers. Kem Ind **61** (2012) 4.
7. Macan B. The new Web of Knowledge 5.0 platform and news about bibliographic and citation database Web of Science. Kem Ind **61** (2012) 32.

Notes

Nikola Tesla
1856 - 1943

Ruđer Bošković
1711 - 1787

Institut Ruđer Bošković



The Ruđer Bošković Institute is the largest Croatian research centre dedicated to fundamental and applied science research. More than 500 academic staff and graduate students work on an array of scientific problems in a multi-disciplinary environment. In Croatia, the RBI is the premiere national institution dedicated to research, higher education and the provision of scientific and technical support to academia, state and local governments and technology based industries. The RBI is part of the EU European Research Area and participates in numerous international collaborations with research institutes and universities sharing the same values and vision.